

# Search history

Ward 10/670031

07/28/2006

=> d his full

(FILE 'HOME' ENTERED AT 14:24:44 ON 28 JUL 2006)

FILE 'REGISTRY' ENTERED AT 14:24:49 ON 28 JUL 2006

L1 886180 SEA ABB=ON PLU=ON (NC4/ESS AND NRS>2 AND N>1 AND (>1 Q/REL))

L2 672553 SEA ABB=ON PLU=ON L1 AND NRRS>1

L3 STRUCTURE UPLOADED

L4 1 SEA SUB=L1 SSS SAM L3

D SCA

L5 174 SEA SUB=L1 SSS FUL L3

SAVE TEMP L5 WAR031STRA/A

FILE 'HCAPLUS' ENTERED AT 14:36:26 ON 28 JUL 2006

L6 58 SEA ABB=ON PLU=ON L5

FILE 'REGISTRY' ENTERED AT 14:36:35 ON 28 JUL 2006

FILE 'STNGUIDE' ENTERED AT 14:39:26 ON 28 JUL 2006

FILE 'REGISTRY' ENTERED AT 14:41:00 ON 28 JUL 2006

L7 STRUCTURE UPLOADED

L8 7 SEA SUB=L5 SSS SAM L7

D SCA

L9 106 SEA SUB=L5 SSS FUL L7

L10 68 SEA ABB=ON PLU=ON L5 NOT L9

FILE 'HCAPLUS' ENTERED AT 14:44:53 ON 28 JUL 2006

L11 8 SEA ABB=ON PLU=ON L10

FILE 'REGISTRY' ENTERED AT 14:45:01 ON 28 JUL 2006

SAVE TEMP L9 WAR031STRNT1/A

FILE 'STNGUIDE' ENTERED AT 14:53:21 ON 28 JUL 2006

FILE 'REGISTRY' ENTERED AT 14:58:12 ON 28 JUL 2006

L12 STRUCTURE UPLOADED

L13 0 SEA SUB=L5 SSS SAM L12

L14 3 SEA SUB=L5 SSS FUL L12

SAVE TEMP WAR031STRB/A L14

D SCA

FILE 'HCAPLUS' ENTERED AT 14:59:46 ON 28 JUL 2006

L15 1 SEA ABB=ON PLU=ON L14

FILE 'BEILSTEIN' ENTERED AT 15:00:01 ON 28 JUL 2006

FILE 'HCAPLUS' ENTERED AT 15:00:12 ON 28 JUL 2006

L16 1 SEA ABB=ON PLU=ON L15 AND L11

L17 60 SEA ABB=ON PLU=ON BULLINGTON J?/AU

L18 3556 SEA ABB=ON PLU=ON FAN X?/AU

L19 1783 SEA ABB=ON PLU=ON JACKSON P?/AU

L20 47109 SEA ABB=ON PLU=ON ZHANG Y?/AU

L21 3 SEA ABB=ON PLU=ON L17 AND (L18 OR L19 OR L20)

L22 138 SEA ABB=ON PLU=ON L18 AND (L19 OR L20)

L23 4 SEA ABB=ON PLU=ON L19 AND L20

L24 138 SEA ABB=ON PLU=ON L18 AND L20

L25 2 SEA ABB=ON PLU=ON L18 AND L19

L26 2 SEA ABB=ON PLU=ON L24 AND (L17 OR L19)

FILE 'BEILSTEIN' ENTERED AT 15:03:41 ON 28 JUL 2006

FILE 'HCAPLUS' ENTERED AT 15:03:46 ON 28 JUL 2006

L27 6 SEA ABB=ON PLU=ON (L21 OR L23 OR L25 OR L26)  
L28 1 SEA ABB=ON PLU=ON L27 AND (L16 OR L11)  
D SCA

FILE 'BEILSTEIN' ENTERED AT 15:04:52 ON 28 JUL 2006

L29 0 SEA SSS SAM L3  
L30 0 SEA ABB=ON PLU=ON (NC4/ESS AND NRS>2 AND N>1 )  
L31 0 SEA SSS SAM L12  
L32 0 SEA SSS FUL L12

FILE 'MARPAT' ENTERED AT 15:07:07 ON 28 JUL 2006

L33 0 SEA SSS SAM L12  
L34 1 SEA SSS FUL L12  
D SCA

FILE 'REGISTRY' ENTERED AT 15:08:33 ON 28 JUL 2006

FILE 'HCAPLUS' ENTERED AT 15:08:36 ON 28 JUL 2006

FILE 'STNGUIDE' ENTERED AT 15:08:47 ON 28 JUL 2006

FILE 'REGISTRY' ENTERED AT 15:08:57 ON 28 JUL 2006

D STAT QUE L5  
D STAT QUE L9  
D STAT QUE L14

FILE 'HCAPLUS' ENTERED AT 15:09:55 ON 28 JUL 2006

D QUE NOS L21  
D QUE NOS L23  
D QUE NOS L25  
D QUE NOS L26  
D QUE NOS L28  
L35 6 SEA ABB=ON PLU=ON L21 OR L23 OR L25 OR L26 OR L28

FILE 'MEDLINE, EMBASE, BIOSIS' ENTERED AT 15:12:13 ON 28 JUL 2006

FILE 'STNGUIDE' ENTERED AT 15:12:17 ON 28 JUL 2006

FILE 'MEDLINE' ENTERED AT 15:12:34 ON 28 JUL 2006

L36 4 SEA ABB=ON PLU=ON (L17 AND (L18 OR L19 OR L20)) OR (L19 AND  
((L17 OR L18) OR L20)) OR (L18 AND L20 AND (L17 OR L19))

FILE 'EMBASE' ENTERED AT 15:13:54 ON 28 JUL 2006

L37 3 SEA ABB=ON PLU=ON (L17 AND (L18 OR L19 OR L20)) OR (L19 AND  
((L17 OR L18) OR L20)) OR (L18 AND L20 AND (L17 OR L19))

FILE 'BIOSIS' ENTERED AT 15:14:06 ON 28 JUL 2006

L38 3 SEA ABB=ON PLU=ON (L17 AND (L18 OR L19 OR L20)) OR (L19 AND  
((L17 OR L18) OR L20)) OR (L18 AND L20 AND (L17 OR L19))

FILE 'WPIX' ENTERED AT 15:14:24 ON 28 JUL 2006

L39 1 SEA ABB=ON PLU=ON (L17 AND (L18 OR L19 OR L20)) OR (L19 AND  
((L17 OR L18) OR L20)) OR (L18 AND L20 AND (L17 OR L19))  
L40 0 SEA SSS SAM L3  
L41 0 SEA SSS SAM L12  
L42 2 SEA SSS FUL L12

SEL SDCN  
EDIT E1-E2 /SDCN /DCN  
L43 1 SEA ABB=ON PLU=ON (RADZT1/DCN OR RADZT3/DCN)  
SEL DCSE L42  
EDIT E3-E4 /DCSE /DCRE  
L44 1 SEA ABB=ON PLU=ON (888697-0-0-0/DCRE OR 888700-0-0-0/DCRE)  
L45 1 SEA ABB=ON PLU=ON L42/DCR  
L46 1 SEA ABB=ON PLU=ON (L43 OR L44 OR L45)  
L47 1 SEA ABB=ON PLU=ON L39 AND L46

FILE 'STNGUIDE' ENTERED AT 15:18:30 ON 28 JUL 2006

FILE 'MEDLINE' ENTERED AT 15:19:08 ON 28 JUL 2006  
D QUE L36

FILE 'EMBASE' ENTERED AT 15:19:22 ON 28 JUL 2006  
D QUE L37

FILE 'BIOSIS' ENTERED AT 15:19:34 ON 28 JUL 2006  
D QUE L38

FILE 'WPIX' ENTERED AT 15:19:47 ON 28 JUL 2006  
D QUE L39  
D QUE L47

L48 1 SEA ABB=ON PLU=ON L39 OR L47

FILE 'STNGUIDE' ENTERED AT 15:20:50 ON 28 JUL 2006

FILE 'HCAPLUS, MEDLINE, EMBASE, BIOSIS, WPIX' ENTERED AT 15:21:15 ON 28 JUL 2006

L49 6 DUP REM L35 L36 L37 L38 L48 (11 DUPLICATES REMOVED)  
ANSWERS '1-6' FROM FILE HCAPLUS  
D IBIB ABS HITSTR L49 1-6

FILE 'STNGUIDE' ENTERED AT 15:22:05 ON 28 JUL 2006

FILE 'REGISTRY' ENTERED AT 15:22:17 ON 28 JUL 2006

FILE 'HCAPLUS' ENTERED AT 15:22:51 ON 28 JUL 2006  
D STAT QUE L16

FILE 'BEILSTEIN' ENTERED AT 15:23:08 ON 28 JUL 2006  
D STAT QUE L32

FILE 'MARPAT' ENTERED AT 15:23:32 ON 28 JUL 2006  
D STAT QUE L34

FILE 'WPIX' ENTERED AT 15:23:45 ON 28 JUL 2006  
D STAT QUE L46

L50 FILE 'HCAPLUS, MARPAT, WPIX' ENTERED AT 15:24:48 ON 28 JUL 2006  
1 DUP REM L16 L32 L34 L46 (2 DUPLICATES REMOVED)  
ANSWER '1' FROM FILE HCAPLUS  
D IBIB ABS HITSTR L50 1

FILE 'STNGUIDE' ENTERED AT 15:25:22 ON 28 JUL 2006

FILE 'HCAPLUS' ENTERED AT 15:25:35 ON 28 JUL 2006

FILE 'REGISTRY' ENTERED AT 15:25:46 ON 28 JUL 2006

L51 D STAT QUE L11  
65 SEA ABB=ON PLU=ON L11 NOT L16

FILE 'STNGUIDE' ENTERED AT 15:26:45 ON 28 JUL 2006

L52 FILE 'HCAPLUS' ENTERED AT 15:26:59 ON 28 JUL 2006  
7 SEA ABB=ON PLU=ON L11 NOT L16  
D IBIB ABS HITSTR L52 1-7

FILE HOME

FILE REGISTRY

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 27 JUL 2006 HIGHEST RN 896463-29-9  
DICTIONARY FILE UPDATES: 27 JUL 2006 HIGHEST RN 896463-29-9

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 6, 2006

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

FILE HCAPLUS

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FILE COVERS 1907 - 28 Jul 2006 VOL 145 ISS 6  
FILE LAST UPDATED: 27 Jul 2006 (20060727/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

FILE STNGUIDE

FILE CONTAINS CURRENT INFORMATION.

LAST RELOADED: Jul 21, 2006 (20060721/UP).

FILE BEILSTEIN

FILE LAST UPDATED ON JUNE 16, 2006

FILE COVERS 1771 TO 2006.

FILE CONTAINS 9,606,495 SUBSTANCES

>>>PLEASE NOTE: Reaction Data and substance data are stored in separate documents and can not be searched together in one query. Reaction data for BEILSTEIN compounds may be displayed immediately with the display codes PRE (preparations) and REA (reactions). A substance answer set retrieved after the search for a chemical name, a compounds with available reaction information by combining with PRE/FA, REA/FA or more generally with RX/FA. The BEILSTEIN Registry Number (BRN) is the link between a BEILSTEIN compound and belonging reactions. For more detailed reaction searches BRNs can be searched as reaction partner BRNs Reactant BRN (RX.RBRN) or Product BRN (RX.PBRN).<<<

>>> FOR SEARCHING PREPARATIONS SEE HELP PRE <<<

\*\*\*\*\*  
\* PLEASE NOTE THAT THERE ARE NO FORMATS FREE OF COST. \*  
\* SET NOTICE FEATURE: THE COST ESTIMATES CALCULATED FOR SET NOTICE \*  
\* ARE BASED ON THE HIGHEST PRICE CATEGORY. THEREFORE; THESE \*  
\* ESTIMATES MAY NOT REFLECT THE ACTUAL COSTS. \*  
\* FOR PRICE INFORMATION SEE HELP COST \*  
\*\*\*\*\*

NEW

\* PATENT NUMBERS (PN) AND BABS ACCESSION NUMBERS (BABSAN) CAN NOW BE SEARCHED, SELECTED AND TRANSFERRED.  
\* NEW DISPLAY FORMATS ALLREF, ALLP AND BABSAN SHOW ALL REFERENCES, ALL PATENT REFERENCES, OR ALL BABS ACCESSION NUMBERS FOR A COMPOUND AT A GLANCE.

FILE MARPAT

FILE CONTENT: 1961-PRESENT VOL 144 ISS 26 (20060721/ED)

SOME MARPAT RECORDS ARE DERIVED FROM INPI DATA FOR 1961-1987

MOST RECENT CITATIONS FOR PATENTS FROM MAJOR ISSUING AGENCIES (COVERAGE TO THESE DATES IS NOT COMPLETE):

US	2006118302	08 JUN 2006
DE	102004054303	11 MAY 2006
EP	1657292	17 MAY 2006
JP	2006120460	11 MAY 2006
WO	2006053912	26 MAY 2006
GB	2419594	03 MAY 2006
FR	2877567	12 MAY 2006
RU	2275374	27 APR 2006
CA	2518664	10 MAR 2006

Expanded G-group definition display now available.

New CAS Information Use Policies, enter HELP USAGETERMS for details.

FILE MEDLINE

FILE LAST UPDATED: 27 Jul 2006 (20060727/UP). FILE COVERS 1950 TO DATE.

On December 11, 2005, the 2006 MeSH terms were loaded.

The MEDLINE reload for 2006 is now (26 Feb.) available. For details

on the 2006 reload, enter HELP RLOAD at an arrow prompt (=>).  
See also:

<http://www.nlm.nih.gov/mesh/>  
[http://www.nlm.nih.gov/pubs/techbull/nd04/nd04\\_mesh.html](http://www.nlm.nih.gov/pubs/techbull/nd04/nd04_mesh.html)  
[http://www.nlm.nih.gov/pubs/techbull/nd05/nd05\\_med\\_data\\_changes.html](http://www.nlm.nih.gov/pubs/techbull/nd05/nd05_med_data_changes.html)  
[http://www.nlm.nih.gov/pubs/techbull/nd05/nd05\\_2006\\_MeSH.html](http://www.nlm.nih.gov/pubs/techbull/nd05/nd05_2006_MeSH.html)

OLDMEDLINE is covered back to 1950.

MEDLINE thesauri in the /CN, /CT, and /MN fields incorporate the MeSH 2006 vocabulary.

This file contains CAS Registry Numbers for easy and accurate substance identification.

#### FILE EMBASE

FILE COVERS 1974 TO 28 Jul 2006 (20060728/ED)

EMBASE has been reloaded. Enter HELP RLOAD for details.

EMBASE is now updated daily. SDI frequency remains weekly (default) and biweekly.

This file contains CAS Registry Numbers for easy and accurate substance identification.

#### FILE BIOSIS

FILE COVERS 1969 TO DATE.

CAS REGISTRY NUMBERS AND CHEMICAL NAMES (CNs) PRESENT  
FROM JANUARY 1969 TO DATE.

RECORDS LAST ADDED: 26 July 2006 (20060726/ED)

#### FILE WPIX

FILE LAST UPDATED: 24 JUL 2006 <20060724/UP>  
MOST RECENT DERWENT UPDATE: 200647 <200647/DW>  
DERWENT WORLD PATENTS INDEX SUBSCRIBER FILE, COVERS 1963 TO DATE

>>> FOR A COPY OF THE DERWENT WORLD PATENTS INDEX STN USER GUIDE,  
PLEASE VISIT:  
[http://www.stn-international.de/training\\_center/patents/stn\\_guide.pdf](http://www.stn-international.de/training_center/patents/stn_guide.pdf) <

>>> FOR DETAILS OF THE PATENTS COVERED IN CURRENT UPDATES, SEE  
<http://scientific.thomson.com/support/patents/coverage/latestupdates/>

>>> PLEASE BE AWARE OF THE NEW IPC REFORM IN 2006, SEE  
[http://www.stn-international.de/stndatabases/details/ipc\\_reform.html](http://www.stn-international.de/stndatabases/details/ipc_reform.html) and  
<http://scientific.thomson.com/media/scpdf/ipcrdwpf.pdf> <<<

>>> FOR FURTHER DETAILS ON THE FORTHCOMING DERWENT WORLD PATENTS  
INDEX ENHANCEMENTS PLEASE VISIT:  
[http://www.stn-international.de/stndatabases/details/dwpi\\_r.html](http://www.stn-international.de/stndatabases/details/dwpi_r.html) <<<

=>

=> file registry

FILE 'REGISTRY' ENTERED AT 15:08:57 ON 28 JUL 2006

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 27 JUL 2006 HIGHEST RN 896463-29-9

DICTIONARY FILE UPDATES: 27 JUL 2006 HIGHEST RN 896463-29-9

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 6, 2006

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

=> d stat que L5

L1 886180 SEA FILE=REGISTRY ABB=ON PLU=ON (NC4/ESS AND NRS>2 AND N>1  
AND (>1 Q/REL))

L3 STR

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

Structure attributes must be viewed using STN Express query preparation.

L5 174 SEA FILE=REGISTRY SUB=L1 SSS FUL L3

100.0% PROCESSED 886160 ITERATIONS  
SEARCH TIME: 00.00.15

174 ANSWERS

STRUCTURE  
QUERY(S)

=> d stat que L9

L1 886180 SEA FILE=REGISTRY ABB=ON PLU=ON (NC4/ESS AND NRS>2 AND N>1  
AND (>1 Q/REL))

L3 STR

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

Structure attributes must be viewed using STN Express query preparation.

L5 174 SEA FILE=REGISTRY SUB=L1 SSS FUL L3

L7 STR

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

Structure attributes must be viewed using STN Express query preparation.

L9 106 SEA FILE=REGISTRY SUB=L5 SSS FUL L7

100.0% PROCESSED 174 ITERATIONS  
SEARCH TIME: 00.00.02

106 ANSWERS

← "Not" structure

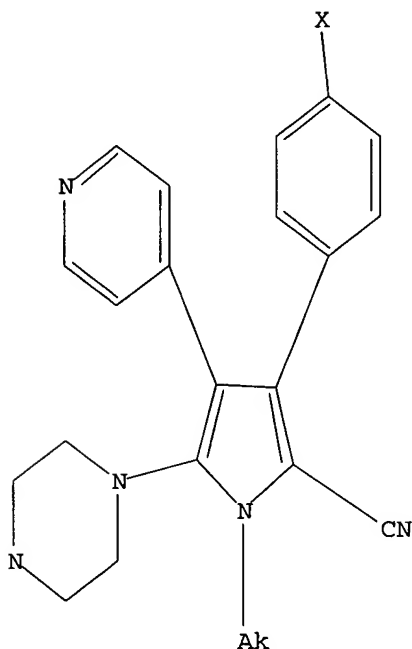
=> d stat que L14

L1 886180 SEA FILE=REGISTRY ABB=ON PLU=ON (NC4/ESS AND NRS>2 AND N>1  
AND (>1 Q/REL))  
L3 STR

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

Structure attributes must be viewed using STN Express query preparation.

L5 174 SEA FILE=REGISTRY SUB=L1 SSS FUL L3  
L12 STR



Structure attributes must be viewed using STN Express query preparation.

L14 3 SEA FILE=REGISTRY SUB=L5 SSS FUL L12

*narrow structure*

100.0% PROCESSED 9 ITERATIONS  
SEARCH TIME: 00.00.01

3 ANSWERS

=> file hcaplus

FILE 'HCAPLUS' ENTERED AT 15:09:55 ON 28 JUL 2006

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

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*AUTHOR  
SEARCH*

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FILE COVERS 1907 - 28 Jul 2006 VOL 145 ISS 6  
FILE LAST UPDATED: 27 Jul 2006 (20060727/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

'OBI' IS DEFAULT SEARCH FIELD FOR 'HCAPLUS' FILE

=> d que nos L21

L17	60	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON	BULLINGTON J?/AU
L18	3556	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON	FAN X?/AU
L19	1783	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON	JACKSON P?/AU
L20	47109	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON	ZHANG Y?/AU
L21	3	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON	L17 AND (L18 OR L19 OR L20)

=> d que nos L23

L19	1783	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON	JACKSON P?/AU
L20	47109	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON	ZHANG Y?/AU
L23	4	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON	L19 AND L20

=> d que nos L25

L18	3556	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON	FAN X?/AU
L19	1783	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON	JACKSON P?/AU
L25	2	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON	L18 AND L19

=> d que nos L26

L17	60	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON	BULLINGTON J?/AU
L18	3556	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON	FAN X?/AU
L19	1783	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON	JACKSON P?/AU
L20	47109	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON	ZHANG Y?/AU
L24	138	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON	L18 AND L20
L26	2	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON	L24 AND (L17 OR L19)

=> d que nos L28

L1	886180	SEA	FILE=REGISTRY	ABB=ON	PLU=ON	(NC4/ESS AND NRS>2 AND N>1 AND (>1 Q/REL))
L3		STR				
L5	174	SEA	FILE=REGISTRY	SUB=L1	SSS FUL	L3
L7		STR				
L9	106	SEA	FILE=REGISTRY	SUB=L5	SSS FUL	L7
L10	68	SEA	FILE=REGISTRY	ABB=ON	PLU=ON	L5 NOT L9
L11	8	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON	L10
L12		STR				
L14	3	SEA	FILE=REGISTRY	SUB=L5	SSS FUL	L12
L15	1	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON	L14
L16	1	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON	L15 AND L11
L17	60	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON	BULLINGTON J?/AU
L18	3556	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON	FAN X?/AU
L19	1783	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON	JACKSON P?/AU
L20	47109	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON	ZHANG Y?/AU
L21	3	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON	L17 AND (L18 OR L19 OR L20)

```
L23      4 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L19 AND L20
L24     138 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L18 AND L20
L25      2 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L18 AND L19
L26      2 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L24 AND (L17 OR L19)
L27      6 SEA FILE=HCAPLUS ABB=ON  PLU=ON  (L21 OR L23 OR L25 OR L26)
L28      1 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L27 AND (L16 OR L11)
```

```
=> s L21 or L23 or L25 or L26 or L28
L35      6 L21 OR L23 OR L25 OR L26 OR L28
```

```
=> => file medline
FILE 'MEDLINE' ENTERED AT 15:19:08 ON 28 JUL 2006
```

FILE LAST UPDATED: 27 Jul 2006 (20060727/UP). FILE COVERS 1950 TO DATE.

On December 11, 2005, the 2006 MeSH terms were loaded.

The MEDLINE reload for 2006 is now (26 Feb.) available. For details on the 2006 reload, enter HELP RLOAD at an arrow prompt (=>). See also:

```
http://www.nlm.nih.gov/mesh/
http://www.nlm.nih.gov/pubs/techbull/nd04/nd04_mesh.html
http://www.nlm.nih.gov/pubs/techbull/nd05/nd05_med_data_changes.html
http://www.nlm.nih.gov/pubs/techbull/nd05/nd05_2006_MeSH.html
```

OLDMEDLINE is covered back to 1950.

MEDLINE thesauri in the /CN, /CT, and /MN fields incorporate the MeSH 2006 vocabulary.

This file contains CAS Registry Numbers for easy and accurate substance identification.

```
=> d que L36
L17      60 SEA FILE=HCAPLUS ABB=ON  PLU=ON  BULLINGTON J?/AU
L18     3556 SEA FILE=HCAPLUS ABB=ON  PLU=ON  FAN X?/AU
L19     1783 SEA FILE=HCAPLUS ABB=ON  PLU=ON  JACKSON P?/AU
L20    47109 SEA FILE=HCAPLUS ABB=ON  PLU=ON  ZHANG Y?/AU
L36      4 SEA FILE=MEDLINE ABB=ON  PLU=ON  (L17 AND (L18 OR L19 OR L20))
      OR (L19 AND ((L17 OR L18) OR L20)) OR (L18 AND L20 AND (L17 OR
      L19))
```

```
=> file embase
FILE 'EMBASE' ENTERED AT 15:19:22 ON 28 JUL 2006
Copyright (c) 2006 Elsevier B.V. All rights reserved.
```

FILE COVERS 1974 TO 28 Jul 2006 (20060728/ED)

EMBASE has been reloaded. Enter HELP RLOAD for details.

EMBASE is now updated daily. SDI frequency remains weekly (default) and biweekly.

This file contains CAS Registry Numbers for easy and accurate substance identification.

```
=> d que L37
```

L17 60 SEA FILE=HCAPLUS ABB=ON PLU=ON BULLINGTON J?/AU  
L18 3556 SEA FILE=HCAPLUS ABB=ON PLU=ON FAN X?/AU  
L19 1783 SEA FILE=HCAPLUS ABB=ON PLU=ON JACKSON P?/AU  
L20 47109 SEA FILE=HCAPLUS ABB=ON PLU=ON ZHANG Y?/AU  
L37 3 SEA FILE=EMBASE ABB=ON PLU=ON (L17 AND (L18 OR L19 OR L20))  
OR (L19 AND ((L17 OR L18) OR L20)) OR (L18 AND L20 AND (L17 OR  
L19))

=> file biosis

FILE 'BIOSIS' ENTERED AT 15:19:34 ON 28 JUL 2006

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FILE COVERS 1969 TO DATE.

CAS REGISTRY NUMBERS AND CHEMICAL NAMES (CNs) PRESENT  
FROM JANUARY 1969 TO DATE.

RECORDS LAST ADDED: 26 July 2006 (20060726/ED)

=> d que L38

L17 60 SEA FILE=HCAPLUS ABB=ON PLU=ON BULLINGTON J?/AU  
L18 3556 SEA FILE=HCAPLUS ABB=ON PLU=ON FAN X?/AU  
L19 1783 SEA FILE=HCAPLUS ABB=ON PLU=ON JACKSON P?/AU  
L20 47109 SEA FILE=HCAPLUS ABB=ON PLU=ON ZHANG Y?/AU  
L38 3 SEA FILE=BIOSIS ABB=ON PLU=ON (L17 AND (L18 OR L19 OR L20))  
OR (L19 AND ((L17 OR L18) OR L20)) OR (L18 AND L20 AND (L17 OR  
L19))

=> file wpix

FILE 'WPIX' ENTERED AT 15:19:47 ON 28 JUL 2006

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FILE LAST UPDATED: 24 JUL 2006 <20060724/UP>

MOST RECENT DERWENT UPDATE: 200647 <200647/DW>

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[http://www.stn-international.de/stndatabases/details/dwpi\\_r.html](http://www.stn-international.de/stndatabases/details/dwpi_r.html) <<<  
'BIX' IS DEFAULT SEARCH FIELD FOR 'WPIX' FILE

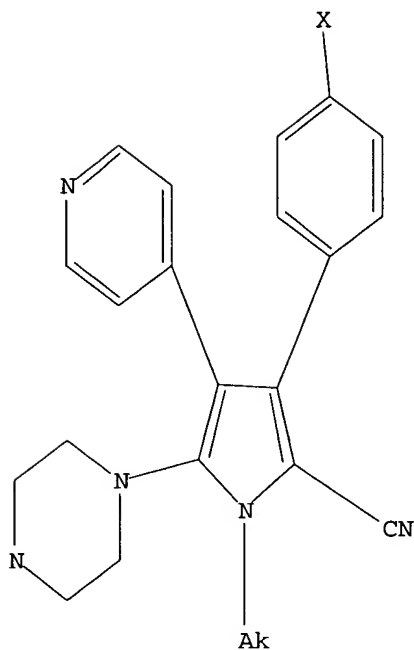
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L17 60 SEA FILE=HCAPLUS ABB=ON PLU=ON BULLINGTON J?/AU  
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L39 1 SEA FILE=WPIX ABB=ON PLU=ON (L17 AND (L18 OR L19 OR L20)) OR

(L19 AND ((L17 OR L18) OR L20)) OR (L18 AND L20 AND (L17 OR L19))

=> d que L47

L12 STR



Structure attributes must be viewed using STN Express query preparation.

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L18     3556 SEA FILE=HCAPLUS ABB=ON  PLU=ON  FAN X?/AU
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L39      1 SEA FILE=WPIX ABB=ON  PLU=ON  (L17 AND (L18 OR L19 OR L20)) OR
        (L19 AND ((L17 OR L18) OR L20)) OR (L18 AND L20 AND (L17 OR
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L42      2 SEA FILE=WPIX SSS FUL L12
L43      1 SEA FILE=WPIX ABB=ON  PLU=ON  (RADZT1/DCN OR RADZT3/DCN)
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        0/DCRE)
L45      1 SEA FILE=WPIX ABB=ON  PLU=ON  L42/DCR
L46      1 SEA FILE=WPIX ABB=ON  PLU=ON  (L43 OR L44 OR L45)
L47      1 SEA FILE=WPIX ABB=ON  PLU=ON  L39 AND L46
  
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=> s L39 or L47

L48 1 L39 OR L47

=> => dup rem L35 L36 L37 L38 L48

FILE 'HCAPLUS' ENTERED AT 15:21:15 ON 28 JUL 2006

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PROCESSING COMPLETED FOR L36  
PROCESSING COMPLETED FOR L37  
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L49 6 DUP REM L35 L36 L37 L38 L48 (11 DUPLICATES REMOVED)  
ANSWERS '1-6' FROM FILE HCAPLUS

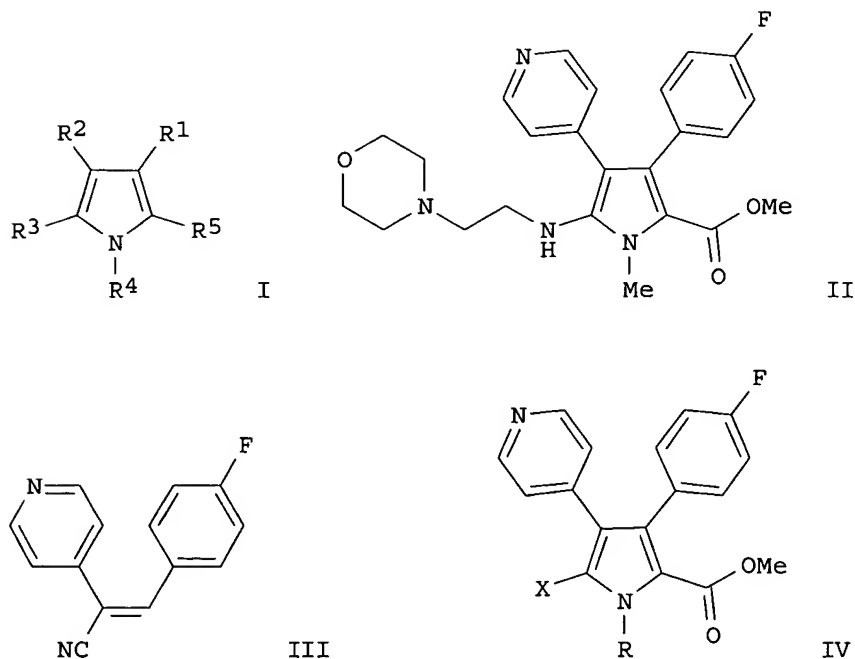
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L49 ANSWER 1 OF 6 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 1  
ACCESSION NUMBER: 2006:453871 HCAPLUS  
TITLE: Synthesis and SAR of  $\alpha$ -sulfonylcarboxylic acids  
as potent matrix metalloproteinase inhibitors  
AUTHOR(S): Zhang, Yue-Mei; Fan, Xiaodong;  
Xiang, Bangping; Chakravarty, Devraj; Scannevin,  
Robert; Burke, Sharon; Karnachi, Prabha; Rhodes,  
Kenneth; Jackson, Paul  
CORPORATE SOURCE: Drug Discovery, Johnson & Johnson Pharmaceutical  
Research and Development, Raritan, NJ, 08869, USA  
SOURCE: Bioorganic & Medicinal Chemistry Letters (2006),  
16(12), 3096-3100  
CODEN: BMCLE8; ISSN: 0960-894X  
PUBLISHER: Elsevier B.V.  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
AB A series of novel carboxylic acid-based  $\alpha$ -sulfone MMP inhibitors  
have been synthesized and the in vitro enzyme SAR is discussed. A  
potential binding mode in the active site of the MMP-9 homol. model was  
highlighted. These compds. are potent MMP-9 inhibitors and are selective  
over MMP-1.  
REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L49 ANSWER 2 OF 6 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 2  
ACCESSION NUMBER: 2004:292020 HCAPLUS  
DOCUMENT NUMBER: 140:321233  
TITLE: A preparation of pyrrole derivatives useful for the  
treatment of disorders ameliorated by reduction of  
TNF- $\alpha$  production and/or p38 activity  
INVENTOR(S): Bullington, James L.; Fan, Xiaodong  
; Jackson, Paul F.; Zhang, Yue-mei  
PATENT ASSIGNEE(S): Janssen Pharmaceutica N.V., Belg.  
SOURCE: PCT Int. Appl., 116 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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WO 2004029040	A1	20040408	WO 2003-US30223	20030924
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RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
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AU 2003278927	A1	20040419	AU 2003-278927	20030924
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EP 1549635	A1	20050706	EP 2003-770442	20030924
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BR 2003014783	A	20050726	BR 2003-14783	20030924
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JP 2006511479	T2	20060406	JP 2004-539896	20030924
NO 2005001967	A	20050621	NO 2005-1967	20050422
PRIORITY APPLN. INFO.:			US 2002-414436P	P 20020927
			WO 2003-US30223	W 20030924
OTHER SOURCE(S):		MARPAT 140:321233		
GI				



AB The invention relates to 3-pyridyl-4-arylpyrrole derivs. of formula I [wherein: R1 and R2 are independently selected from (un)substituted (hetero)aryl; R3 = H, (un)substituted alkyl, -N:CR6-, -C(O)R7, etc.; R4 = H, (un)substituted alkyl, (un)substituted (hetero)aryl, etc.; R5 =

(un)substituted alkyl, C(O)OR<sub>7</sub>, C(O)R<sub>7</sub>, CN, NO<sub>2</sub>, halo, etc.; R<sub>6</sub> and R<sub>7</sub> are independently selected from H, (un)substituted alkyl, (un)substituted aryl, (un)substituted heterocycle; with provisos], and pharmaceutical compns. comprising the same, useful for treating disorders ameliorated by reducing TNF- $\alpha$  production and/or p38 activity in appropriate cells. The invention compds. I were screened for p38 inhibition (in-vitro enzyme assays) and TNF- $\alpha$  inhibition (in-vitro whole cell assays and in vivo rodent assay). The invention also provides therapeutic and prophylactic methods using the instant pharmaceutical compns. For instance, pyrrole derivative II (compound 5; mouse 10 mg/kg, 0.5 h, 44% inhibition of TNF- $\alpha$  production) was prepared via condensation of 4-fluorobenzaldehyde with 4-pyridylacetonitrile, heterocyclization of the obtained pyridine derivative III with Me isocyanoacetate, N-methylation of the pyrrole ring of the obtained pyrrolecarboxylate derivative IV (X = H, R = H), bromination of the pyrrolecarboxylate derivative IV (X = H, R = Me), and subsequent amination of the obtained bromopyrrole derivative IV (X = Br, R = Me) by 4-(2-aminoethyl)morpholine.

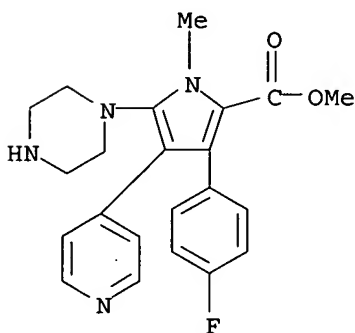
IT 678161-35-8P 678161-52-9P

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(intermediate; preparation of pyridyl(aryl)pyrrole derivs. useful for the treatment of disorders ameliorated by reduction of TNF- $\alpha$  production and/or p38 activity)

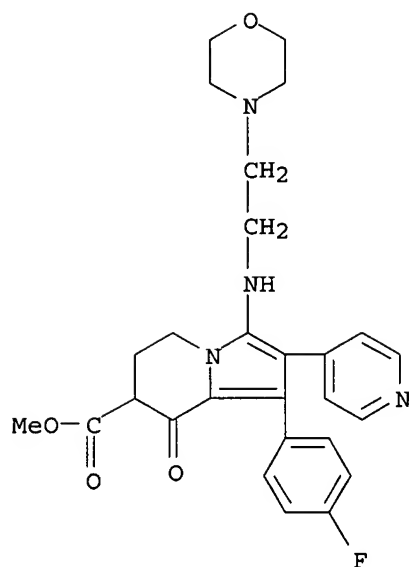
RN 678161-35-8 HCAPLUS

CN 1H-Pyrrole-2-carboxylic acid, 3-(4-fluorophenyl)-1-methyl-5-(1-piperazinyl)-4-(4-pyridinyl)-, methyl ester (9CI) (CA INDEX NAME)



RN 678161-52-9 HCAPLUS

CN 7-Indolizinecarboxylic acid, 1-(4-fluorophenyl)-5,6,7,8-tetrahydro-3-[[2-(4-morpholinyl)ethyl]amino]-8-oxo-2-(4-pyridinyl)-, methyl ester (9CI) (CA INDEX NAME)



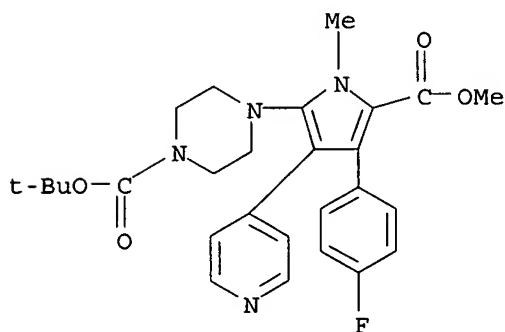
IT 678161-34-7

RL: PAC (Pharmacological activity); RCT (Reactant); THU (Therapeutic use);  
BIOL (Biological study); RACT (Reactant or reagent); USES (Uses)

(preparation of pyridyl(aryl)pyrrole derivs. useful for the treatment of  
disorders ameliorated by reduction of TNF- $\alpha$  production and/or p38  
activity)

RN 678161-34-7 HCAPLUS

CN 1-Piperazinecarboxylic acid, 4-[4-(4-fluorophenyl)-5-(methoxycarbonyl)-1-  
methyl-3-(4-pyridinyl)-1H-pyrrol-2-yl]-, 1,1-dimethylethyl ester (9CI)  
(CA INDEX NAME)



IT 678161-38-1P 678161-40-5P 678161-41-6P  
678161-42-7P 678161-54-1P 678162-27-1P  
678162-29-3P 678162-34-0P 678162-35-1P  
678162-36-2P 678162-37-3P 678162-39-5P  
678162-41-9P 678162-43-1P 678162-45-3P  
678162-46-4P 678162-47-5P 678162-50-0P  
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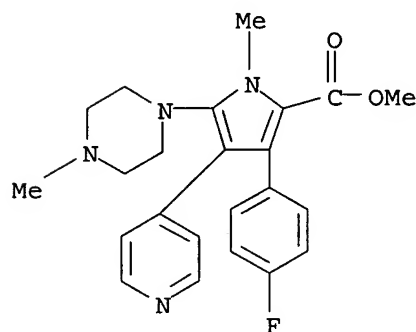
678163-30-9P 678163-33-2P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of pyridyl(aryl)pyrrole derivs. useful for the treatment of disorders ameliorated by reduction of TNF- $\alpha$  production and/or p38 activity)

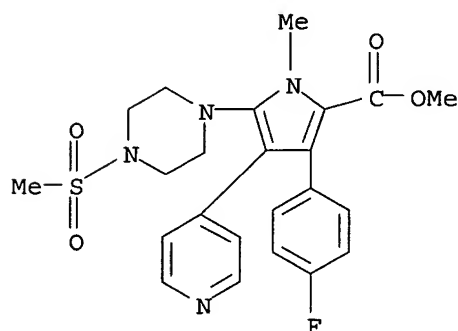
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CN 1H-Pyrrole-2-carboxylic acid, 3-(4-fluorophenyl)-1-methyl-5-(4-methyl-1-piperazinyl)-4-(4-pyridinyl)-, methyl ester (9CI) (CA INDEX NAME)



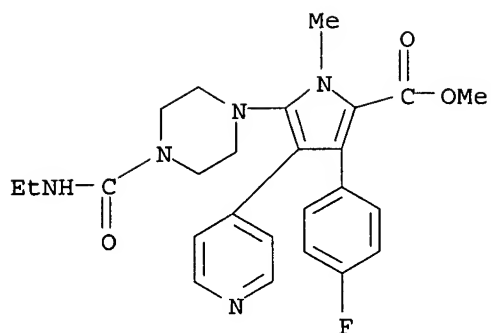
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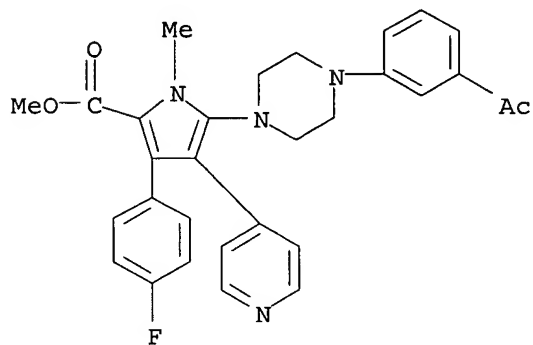
RN 678161-41-6 HCAPLUS

CN 1H-Pyrrole-2-carboxylic acid, 5-[4-[(ethylamino)carbonyl]-1-piperazinyl]-3-(4-fluorophenyl)-1-methyl-4-(4-pyridinyl)-, methyl ester (9CI) (CA INDEX NAME)



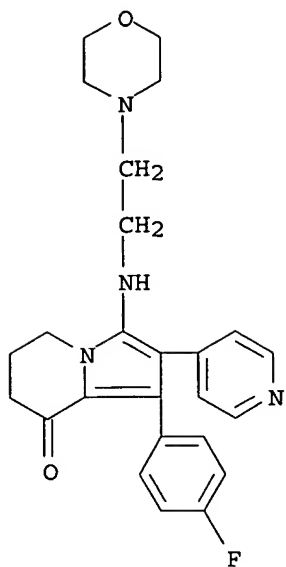
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CN 1H-Pyrrole-2-carboxylic acid, 5-[4-(3-acetylphenyl)-1-piperazinyl]-3-(4-fluorophenyl)-1-methyl-4-(4-pyridinyl)-, methyl ester (9CI) (CA INDEX NAME)



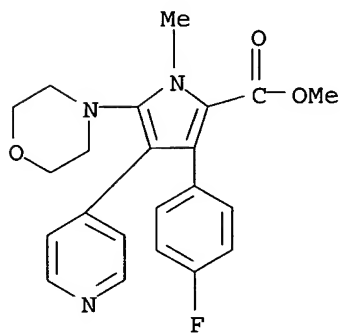
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CN 8(5H)-Indolizinone, 1-(4-fluorophenyl)-6,7-dihydro-3-[[2-(4-morpholinyl)ethyl]amino]-2-(4-pyridinyl)- (9CI) (CA INDEX NAME)



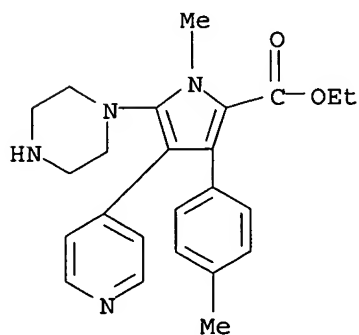
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CN 1H-Pyrrole-2-carboxylic acid, 3-(4-fluorophenyl)-1-methyl-5-(4-morpholinyl)-4-(4-pyridinyl)-, methyl ester (9CI) (CA INDEX NAME)



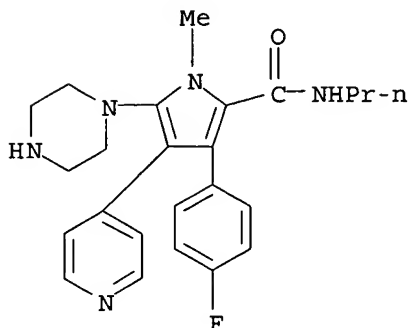
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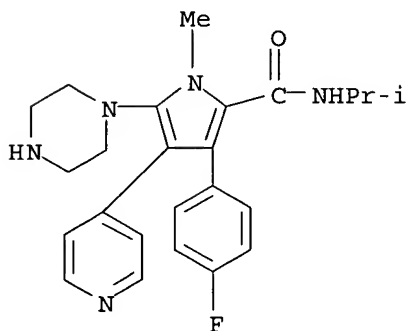
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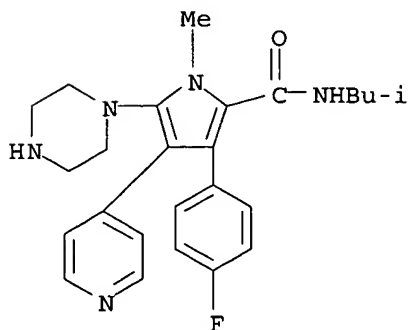
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CN 1H-Pyrrole-2-carboxamide, 3-(4-fluorophenyl)-1-methyl-N-(1-methylethyl)-5-(1-piperazinyl)-4-(4-pyridinyl)- (9CI) (CA INDEX NAME)



RN 678162-36-2 HCAPLUS

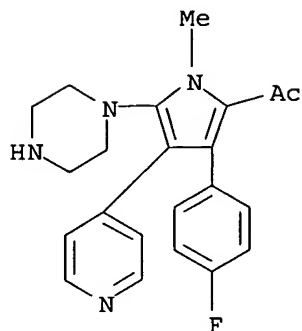
CN 1H-Pyrrole-2-carboxamide, 3-(4-fluorophenyl)-1-methyl-N-(2-methylpropyl)-5-(1-piperazinyl)-4-(4-pyridinyl)- (9CI) (CA INDEX NAME)



RN 678162-37-3 HCAPLUS

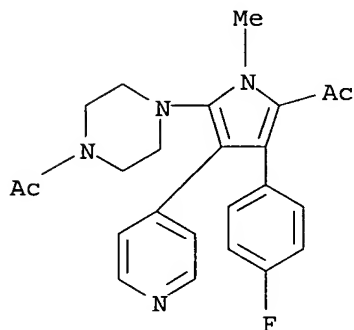
CN Ethanone, 1-[3-(4-fluorophenyl)-1-methyl-5-(1-piperazinyl)-4-(4-pyridinyl)-

1H-pyrrol-2-yl]- (9CI) (CA INDEX NAME)



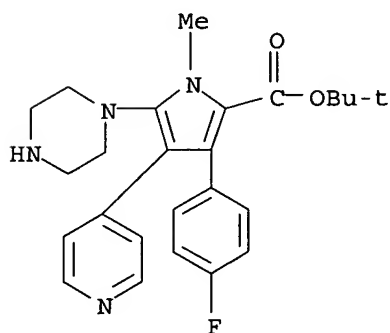
RN 678162-39-5 HCAPLUS

CN Piperazine, 1-acetyl-4-[5-acetyl-4-(4-fluorophenyl)-1-methyl-3-(4-pyridinyl)-1H-pyrrol-2-yl]- (9CI) (CA INDEX NAME)



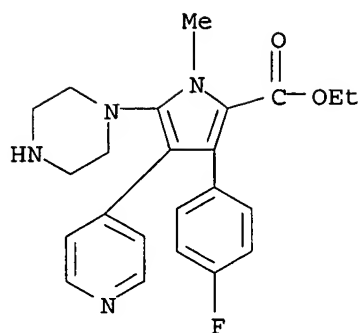
RN 678162-41-9 HCAPLUS

CN 1H-Pyrrole-2-carboxylic acid, 3-(4-fluorophenyl)-1-methyl-5-(1-piperazinyl)-4-(4-pyridinyl)-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



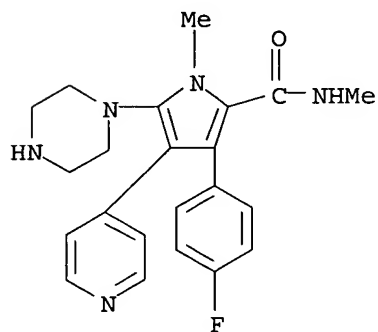
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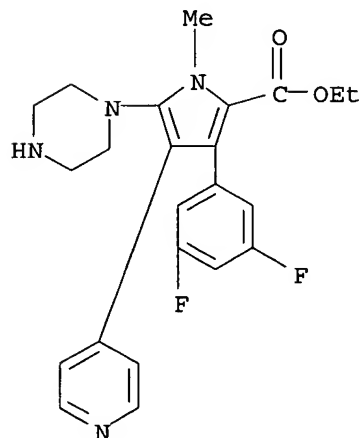
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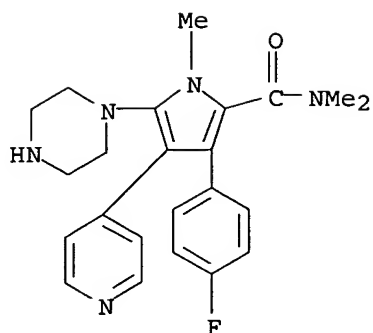
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CN 1H-Pyrrole-2-carboxylic acid, 3-(3,5-difluorophenyl)-1-methyl-5-(1-piperazinyl)-4-(4-pyridinyl)-, ethyl ester (9CI) (CA INDEX NAME)



RN 678162-47-5 HCAPLUS

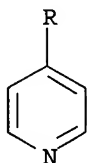
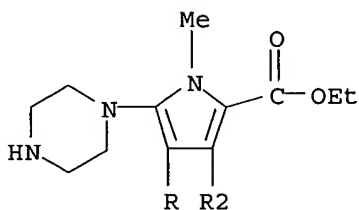
CN 1H-Pyrrole-2-carboxamide, 3-(4-fluorophenyl)-N,N,1-trimethyl-5-(1-piperazinyl)-4-(4-pyridinyl)- (9CI) (CA INDEX NAME)



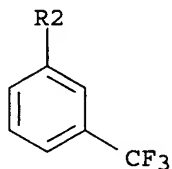
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CN 1H-Pyrrole-2-carboxylic acid, 1-methyl-5-(1-piperazinyl)-4-(4-pyridinyl)-3-[3-(trifluoromethyl)phenyl]-, ethyl ester (9CI) (CA INDEX NAME)

PAGE 1-A



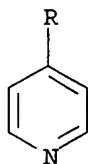
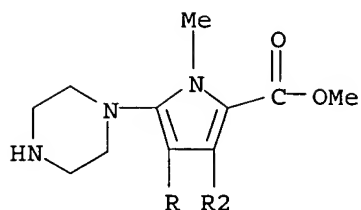
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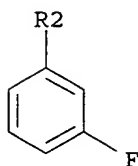
RN 678162-51-1 HCAPLUS

CN 1H-Pyrrole-2-carboxylic acid, 3-(3-fluorophenyl)-1-methyl-5-(1-piperazinyl)-4-(4-pyridinyl)-, methyl ester (9CI) (CA INDEX NAME)

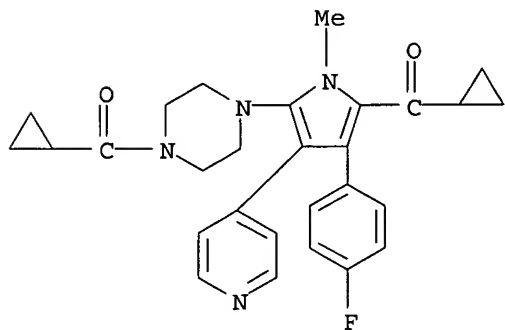
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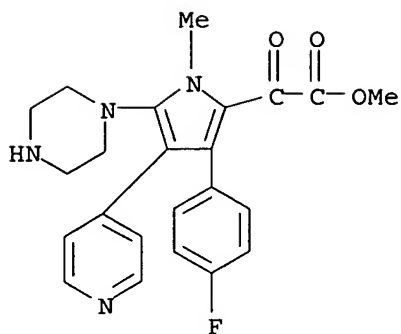


RN 678162-52-2 HCAPLUS  
 CN Piperazine, 1-(cyclopropylcarbonyl)-4-[5-(cyclopropylcarbonyl)-4-(4-fluorophenyl)-1-methyl-3-(4-pyridinyl)-1H-pyrrol-2-yl]- (9CI) (CA INDEX NAME)

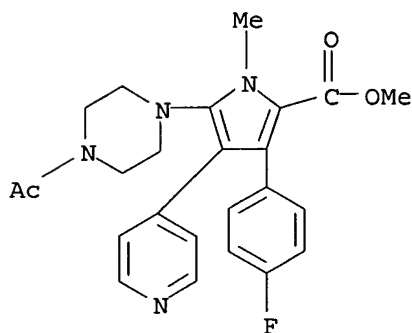


RN 678162-53-3 HCAPLUS  
 CN 1H-Pyrrole-2-acetic acid, 3-(4-fluorophenyl)-1-methyl- $\alpha$ -oxo-5-(1-piperazinyl)-4-(4-pyridinyl)-, methyl ester (9CI) (CA INDEX NAME)

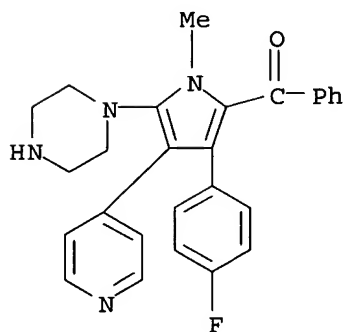




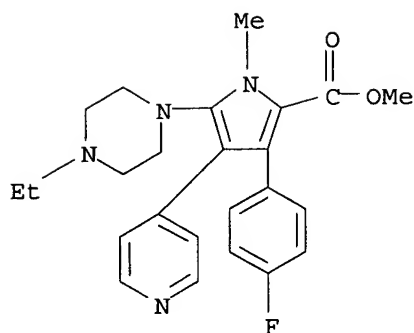
RN 678162-61-3 HCAPLUS  
 CN 1H-Pyrrole-2-carboxylic acid, 5-(4-acetyl-1-piperazinyl)-3-(4-fluorophenyl)-1-methyl-4-(4-pyridinyl)-, methyl ester (9CI) (CA INDEX NAME)



RN 678162-62-4 HCAPLUS  
 CN Methanone, [3-(4-fluorophenyl)-1-methyl-5-(1-piperazinyl)-4-(4-pyridinyl)-1H-pyrrol-2-yl]phenyl- (9CI) (CA INDEX NAME)

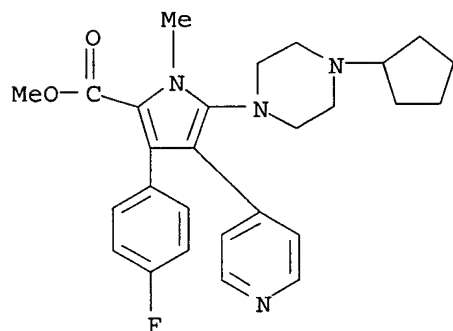


RN 678162-69-1 HCAPLUS  
 CN 1H-Pyrrole-2-carboxylic acid, 5-(4-ethyl-1-piperazinyl)-3-(4-fluorophenyl)-1-methyl-4-(4-pyridinyl)-, methyl ester (9CI) (CA INDEX NAME)



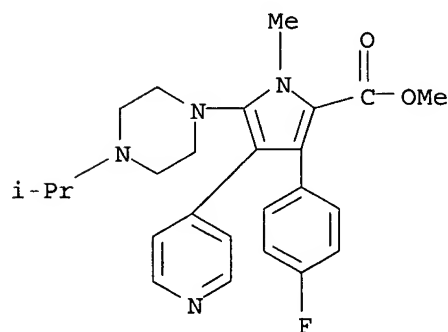
RN 678162-70-4 HCAPLUS

CN 1H-Pyrrole-2-carboxylic acid, 5-(4-cyclopentyl-1-piperazinyl)-3-(4-fluorophenyl)-1-methyl-4-(4-pyridinyl)-, methyl ester (9CI) (CA INDEX NAME)



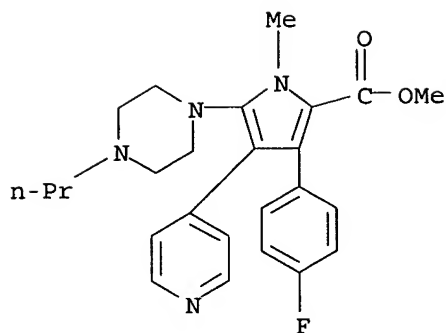
RN 678162-71-5 HCAPLUS

CN 1H-Pyrrole-2-carboxylic acid, 3-(4-fluorophenyl)-1-methyl-5-[4-(1-methylethyl)-1-piperazinyl]-4-(4-pyridinyl)-, methyl ester (9CI) (CA INDEX NAME)



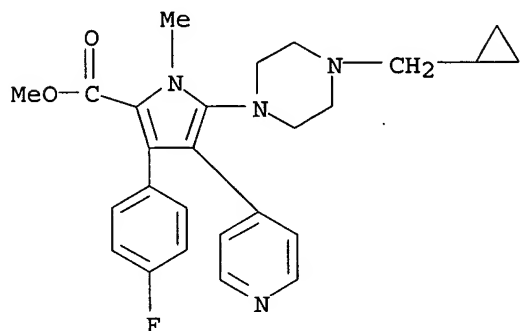
RN 678162-72-6 HCAPLUS

CN 1H-Pyrrole-2-carboxylic acid, 3-(4-fluorophenyl)-1-methyl-5-(4-propyl-1-piperazinyl)-4-(4-pyridinyl)-, methyl ester (9CI) (CA INDEX NAME)



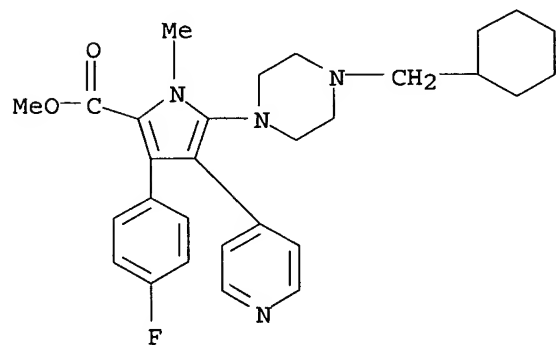
RN 678162-73-7 HCAPLUS

CN 1H-Pyrrole-2-carboxylic acid, 5-[4-(cyclopropylmethyl)-1-piperazinyl]-3-(4-fluorophenyl)-1-methyl-4-(4-pyridinyl)-, methyl ester (9CI) (CA INDEX NAME)



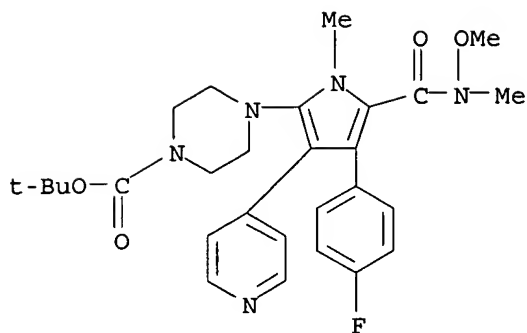
RN 678162-75-9 HCAPLUS

CN 1H-Pyrrole-2-carboxylic acid, 5-[4-(cyclohexylmethyl)-1-piperazinyl]-3-(4-fluorophenyl)-1-methyl-4-(4-pyridinyl)-, methyl ester (9CI) (CA INDEX NAME)



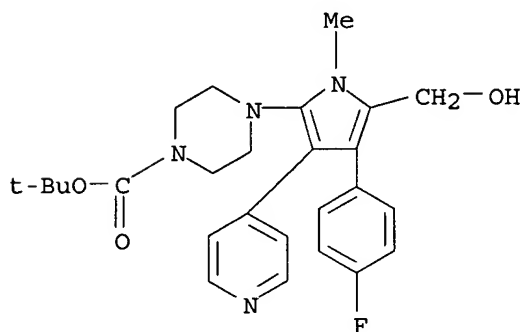
RN 678162-93-1 HCAPLUS

CN 1-Piperazinecarboxylic acid, 4-[4-(4-fluorophenyl)-5-[(methoxymethylamino)carbonyl]-1-methyl-3-(4-pyridinyl)-1H-pyrrol-2-yl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



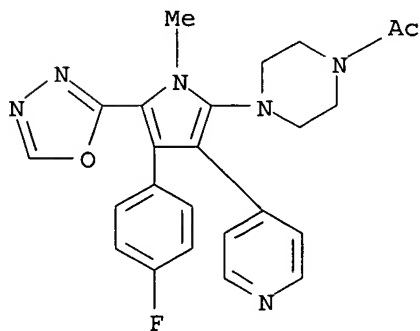
RN 678162-99-7 HCAPLUS

CN 1-Piperazinecarboxylic acid, 4-[4-(4-fluorophenyl)-5-(hydroxymethyl)-1-methyl-3-(4-pyridinyl)-1H-pyrrol-2-yl]-, 1,1-dimethylethyl ester (9CI)  
(CA INDEX NAME)



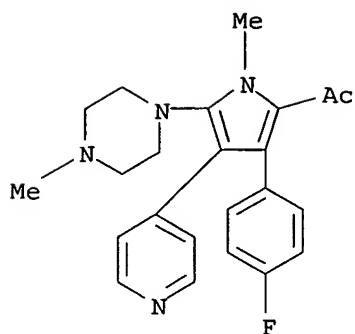
RN 678163-05-8 HCAPLUS

CN Piperazine, 1-acetyl-4-[4-(4-fluorophenyl)-1-methyl-5-(1,3,4-oxadiazol-2-yl)-3-(4-pyridinyl)-1H-pyrrol-2-yl]- (9CI) (CA INDEX NAME)



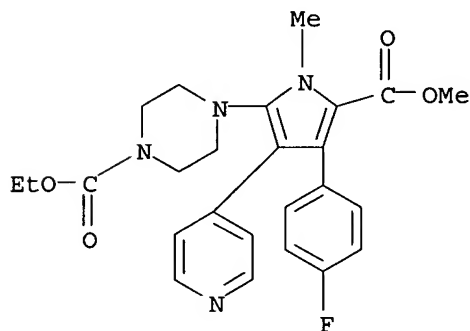
RN 678163-25-2 HCAPLUS

CN Ethanone, 1-[3-(4-fluorophenyl)-1-methyl-5-(4-methyl-1-piperazinyl)-4-(4-pyridinyl)-1H-pyrrol-2-yl]- (9CI) (CA INDEX NAME)



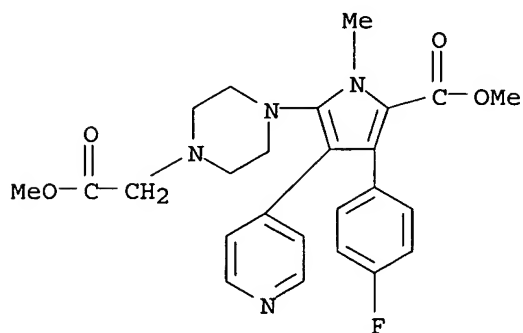
RN 678163-26-3 HCAPLUS

CN 1-Piperazinecarboxylic acid, 4-[4-(4-fluorophenyl)-5-(methoxycarbonyl)-1-methyl-3-(4-pyridinyl)-1H-pyrrol-2-yl]-, ethyl ester (9CI) (CA INDEX NAME)



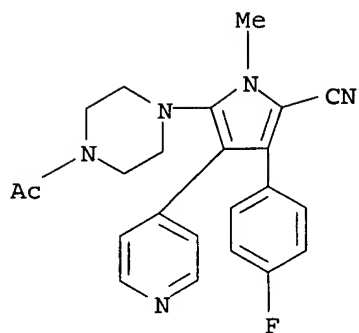
RN 678163-28-5 HCAPLUS

CN 1-Piperazineacetic acid, 4-[4-(4-fluorophenyl)-5-(methoxycarbonyl)-1-methyl-3-(4-pyridinyl)-1H-pyrrol-2-yl]-, methyl ester (9CI) (CA INDEX NAME)



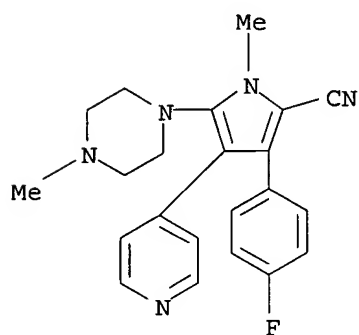
RN 678163-29-6 HCAPLUS

CN Piperazine, 1-acetyl-4-[5-cyano-4-(4-fluorophenyl)-1-methyl-3-(4-pyridinyl)-1H-pyrrol-2-yl]- (9CI) (CA INDEX NAME)



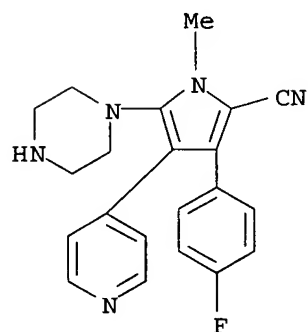
RN 678163-30-9 HCAPLUS

CN 1H-Pyrrole-2-carbonitrile, 3-(4-fluorophenyl)-1-methyl-5-(4-methyl-1-piperazinyl)-4-(4-pyridinyl)- (9CI) (CA INDEX NAME)



RN 678163-33-2 HCAPLUS

CN 1H-Pyrrole-2-carbonitrile, 3-(4-fluorophenyl)-1-methyl-5-(1-piperazinyl)-4-(4-pyridinyl)- (9CI) (CA INDEX NAME)



L49 ANSWER 3 OF 6 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 3

ACCESSION NUMBER: 2004:448213 HCAPLUS

DOCUMENT NUMBER: 140:404063

TITLE: Disruption of CCT $\beta$ 2 expression leads to gonadal dysfunction

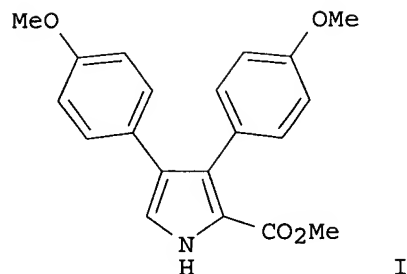
AUTHOR(S): Jackowski, Suzanne; Rehg, Jerold E.; Zhang, Yong-Mei; Wang, Jina; Miller, Karen;

**Jackson, Pam; Karim, Mohammad A.**  
**CORPORATE SOURCE:** Department of Infectious Diseases, St. Jude Children's  
Research Hospital, Memphis, TN, 38105, USA  
**SOURCE:** Molecular and Cellular Biology (2004), 24(11),  
4720-4733  
CODEN: MCEBD4; ISSN: 0270-7306  
**PUBLISHER:** American Society for Microbiology  
**DOCUMENT TYPE:** Journal  
**LANGUAGE:** English  
**AB** There are two mammalian genes that encode isoforms of CTP:phosphocholine  
cytidyltransferase (CCT), a key rate-controlling step in membrane  
phospholipid biogenesis. Quant. determination of the CCT transcripts reveals  
that

CCT $\alpha$  is ubiquitously expressed and is found at the highest levels in  
the testis and lung, with lower levels in the liver and ovary. CCT $\beta$ 2  
is a very minor isoform in most tissues but is significantly expressed in  
the brain, lung, and gonads. CCT $\beta$ 3 is the third isoform recently  
discovered in mice and is expressed in the same tissues as CCT $\beta$ 2,  
with its highest level in testes. We investigated the role(s) of  
CCT $\beta$ 2 by generating knockout mice. The brains and lungs of mice  
lacking CCT $\beta$ 2 expression did not exhibit any overt defects. On the  
other hand, a large percentage of the CCT $\beta$ 2-/- females were sterile  
and their ovaries exhibited defective ovarian follicle development. The  
proportion of female CCT $\beta$ 2-/- mice with defective ovaries increased  
as the animals aged. The rare litters born from CCT $\beta$ 2-/- +  
CCT $\beta$ 2-/- matings had the normal number of pups. The abnormal ovarian  
histopathol. was characterized by disorganization of the tissue in young  
adult mice and absence of follicles and ova in older mice, along with  
interstitial stromal cell hyperplasia which culminated in the emergence of  
tubulostromal ovarian tumors by 16 mo of age. Grossly defective  
CCT $\beta$ 2-/- ovaries were associated with high follicle-stimulating (FSH)  
and luteinizing (LH) hormone levels. Male CCT $\beta$ 2-/- mice exhibited  
progressive multi-focal testicular degeneration and reduced fertility but  
had normal FSH and LH levels. Thus, the most notable phenotype of  
CCT $\beta$ 2 knockout mice was gonad degeneration and reproductive  
deficiency. The results indicate that although CCT $\beta$ 2 is expressed at  
very low levels compared to the  $\alpha$ -isoform, loss of CCT $\beta$ 2  
expression causes a breakdown in the gonadal response to hormonal  
stimulation.

**REFERENCE COUNT:** 67 THERE ARE 67 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L49 ANSWER 4 OF 6 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 4  
**ACCESSION NUMBER:** 2002:917652 HCAPLUS  
**DOCUMENT NUMBER:** 138:137442  
**TITLE:** Regioselective Preparation of 2-Substituted 3,4-Diaryl  
Pyrroles: A Concise Total Synthesis of Ningalin B  
**AUTHOR(S):** Bullington, James L.; Wolff, Russell R.;  
Jackson, Paul F.  
**CORPORATE SOURCE:** Discovery Research, Johnson & Johnson Pharmaceutical  
Research and Development, L.L.C., Raritan, NJ, 08869,  
USA  
**SOURCE:** Journal of Organic Chemistry (2002), 67(26), 9439-9442  
CODEN: JOCEAH; ISSN: 0022-3263  
**PUBLISHER:** American Chemical Society  
**DOCUMENT TYPE:** Journal  
**LANGUAGE:** English  
**OTHER SOURCE(S):** CASREACT 138:137442  
GI



AB Me isocyanoacetate undergoes a 2 + 3 cycloaddn. with  $\alpha,\beta$ -unsatd. nitriles to provide a regioselective synthesis of 2-substituted 3,4-diaryl pyrroles. The ease of preparation of  $\alpha,\beta$ -unsatd. nitriles allows the rapid synthesis of pyrroles with varied substituents. Using this method, a key intermediate (I) for the synthesis of the marine natural products lukianol A, lamellarin O, and lamellarin Q was prepared in two steps. A total synthesis of ningalin B was also accomplished utilizing this methodol.

REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L49 ANSWER 5 OF 6 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 5

ACCESSION NUMBER: 2002:808686 HCAPLUS

DOCUMENT NUMBER: 138:205007

TITLE: Synthesis of pyrimido[4,5-b]indoles and benzo[4,5]furo[2,3-d]pyrimidines via palladium-catalyzed intramolecular arylation

AUTHOR(S): Zhang, Yue-Mei; Razler, Thomas; Jackson, Paul F.

CORPORATE SOURCE: Johnson & Johnson Pharmaceutical Research and Development, LLC, Raritan, NJ, 08869, USA

SOURCE: Tetrahedron Letters (2002), 43(46), 8235-8239  
CODEN: TELEAY; ISSN: 0040-4039

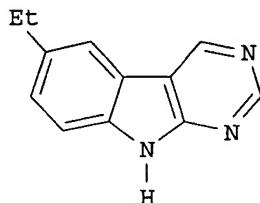
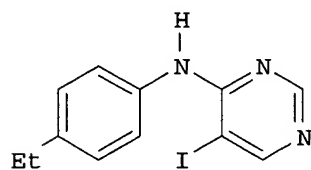
PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 138:205007

GI



AB Various pyrimido[4,5-b]indoles and benzo[4,5]furo[2,3-d]pyrimidines were



synthesized via a palladium-catalyzed intramol. arylation of pyrimidine substrates. Thus, 4-aryloxy- or 4-anilino-5-iodopyrimidines, e.g. I, were treated with Pd(OAc)<sub>2</sub>(PPh<sub>3</sub>)<sub>2</sub> and base in DMF to give the regioselective cyclized heterocycles, e.g. II.

REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L49 ANSWER 6 OF 6 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 6

ACCESSION NUMBER: 2002:607174 HCAPLUS

DOCUMENT NUMBER: 138:162771

TITLE: Pyridinylimidazole based p38 MAP kinase inhibitors

AUTHOR(S): Jackson, Paul F.; Bullington, James

L.

CORPORATE SOURCE: Discovery Research, Johnson and Johnson Pharmaceutical Research and Development, L.L.C., Raritan, NJ, 08869, USA

SOURCE: Current Topics in Medicinal Chemistry (Hilversum, Netherlands) (2002), 2(9), 1011-1020

CODEN: CTMCCL; ISSN: 1568-0266

PUBLISHER: Bentham Science Publishers Ltd.

DOCUMENT TYPE: Journal; General Review

LANGUAGE: English

AB A review. The p38 MAP kinase is thought to be involved in a variety of inflammatory and immunol. disorders such as rheumatoid arthritis. The pyridinylimidazole class of compds. was the first to potently inhibit this kinase. Since the original reports of their efficacy, they have become the most widely studied series of inhibitors of this kinase. This framework has served as a starting point for further synthetic work and several compds. have entered clin. trials. These compds. have also been utilized to elucidate the role of p38 kinase in the immune system, and more recently have been used to examine the role of this kinase in central nervous system disorders.

REFERENCE COUNT: 45 THERE ARE 45 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=&gt; □

# STRUCTURE SEARCH (narrow)

=&gt; file registry

FILE 'REGISTRY' ENTERED AT 15:22:17 ON 28 JUL 2006

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STRUCTURE FILE UPDATES: 27 JUL 2006 HIGHEST RN 896463-29-9

DICTIONARY FILE UPDATES: 27 JUL 2006 HIGHEST RN 896463-29-9

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 6, 2006

Please note that search-term pricing does apply when  
conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and  
predicted properties as well as tags indicating availability of  
experimental property data in the original document. For information  
on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

=&gt; file hcaplus

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FILE COVERS 1907 - 28 Jul 2006 VOL 145 ISS 6

FILE LAST UPDATED: 27 Jul 2006 (20060727/ED)

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This file contains CAS Registry Numbers for easy and accurate  
substance identification.

'OBI' IS DEFAULT SEARCH FIELD FOR 'HCAPLUS' FILE

=&gt; d stat que L16

L1 886180 SEA FILE=REGISTRY ABB=ON PLU=ON (NC4/ESS AND NRS>2 AND N>1  
AND (>1 Q/REL))

L3 STR

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

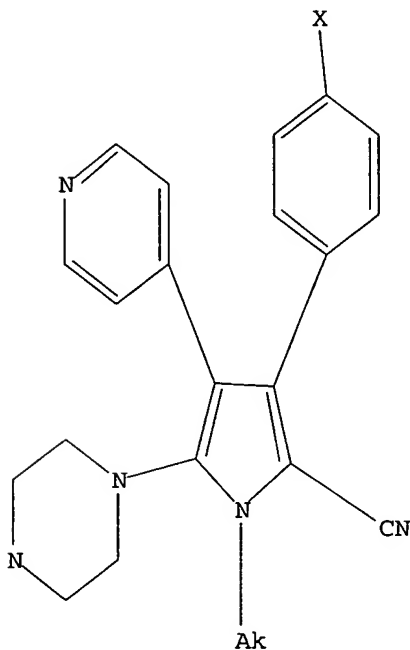
Structure attributes must be viewed using STN Express query preparation.

L5 174 SEA FILE=REGISTRY SUB=L1 SSS FUL L3  
L7 STR

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

Structure attributes must be viewed using STN Express query preparation.

L9 106 SEA FILE=REGISTRY SUB=L5 SSS FUL L7  
L10 68 SEA FILE=REGISTRY ABB=ON PLU=ON L5 NOT L9  
L11 8 SEA FILE=HCAPLUS ABB=ON PLU=ON L10  
L12 STR



Structure attributes must be viewed using STN Express query preparation.

L14 3 SEA FILE=REGISTRY SUB=L5 SSS FUL L12  
L15 1 SEA FILE=HCAPLUS ABB=ON PLU=ON L14  
L16 1 SEA FILE=HCAPLUS ABB=ON PLU=ON L15 AND L11

=> file beilstein

FILE 'BEILSTEIN' ENTERED AT 15:23:08 ON 28 JUL 2006

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FILE LAST UPDATED ON JUNE 16, 2006

FILE COVERS 1771 TO 2006.

\*\*\* FILE CONTAINS 9,606,495 SUBSTANCES \*\*\*

>>>PLEASE NOTE: Reaction Data and substance data are stored in  
separate documents and can not be searched together in one query.  
Reaction data for BEILSTEIN compounds may be displayed  
immediately with the display codes PRE (preparations) and REA

(reactions). A substance answer set retrieved after the search for a chemical name, a compounds with available reaction information by combining with PRE/FA, REA/FA or more generally with RX/FA. The BEILSTEIN Registry Number (BRN) is the link between a BEILSTEIN compound and belonging reactions. For mo detailed reaction searches BRNs can be searched as reaction partner BRNs Reactant BRN (RX.RBRN) or Product BRN (RX.PBRN).<<<

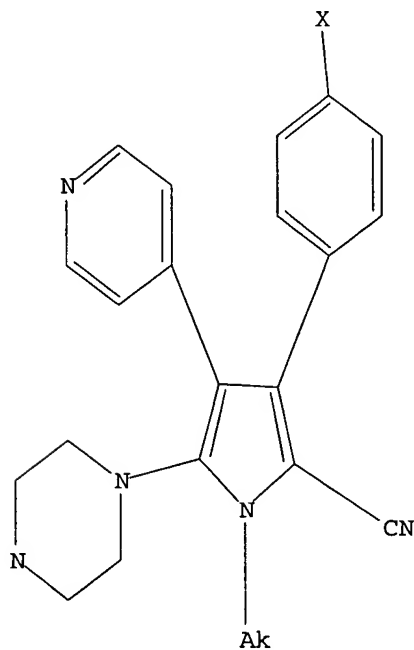
>>> FOR SEARCHING PREPARATIONS SEE HELP PRE <<<

\*\*\*\*\*  
 \* PLEASE NOTE THAT THERE ARE NO FORMATS FREE OF COST. \*  
 \* SET NOTICE FEATURE: THE COST ESTIMATES CALCULATED FOR SET NOTICE \*  
 \* ARE BASED ON THE HIGHEST PRICE CATEGORY. THEREFORE; THESE \*  
 \* ESTIMATES MAY NOT REFLECT THE ACTUAL COSTS. \*  
 \* FOR PRICE INFORMATION SEE HELP COST \*  
 \*\*\*\*\*

#### NEW

\* PATENT NUMBERS (PN) AND BABS ACCESSION NUMBERS (BABSAN) CAN NOW BE SEARCHED, SELECTED AND TRANSFERRED.  
 \* NEW DISPLAY FORMATS ALLREF, ALLP AND BABSAN SHOW ALL REFERENCES, ALL PATENT REFERENCES, OR ALL BABS ACCESSION NUMBERS FOR A COMPOUND AT A GLANCE.

=> d stat que L32  
 L12 STR



Structure attributes must be viewed using STN Express query preparation.  
 L32 0 SEA FILE=BEILSTEIN SSS FUL L12

100.0% PROCESSED 0 ITERATIONS 0 ANSWERS  
 SEARCH TIME: 00.00.02

=> file marpat

FILE 'MARPAT' ENTERED AT 15:23:32 ON 28 JUL 2006

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FILE CONTENT: 1961-PRESENT VOL 144 ISS 26 (20060721/ED)

SOME MARPAT RECORDS ARE DERIVED FROM INPI DATA FOR 1961-1987

MOST RECENT CITATIONS FOR PATENTS FROM MAJOR ISSUING AGENCIES  
(COVERAGE TO THESE DATES IS NOT COMPLETE):

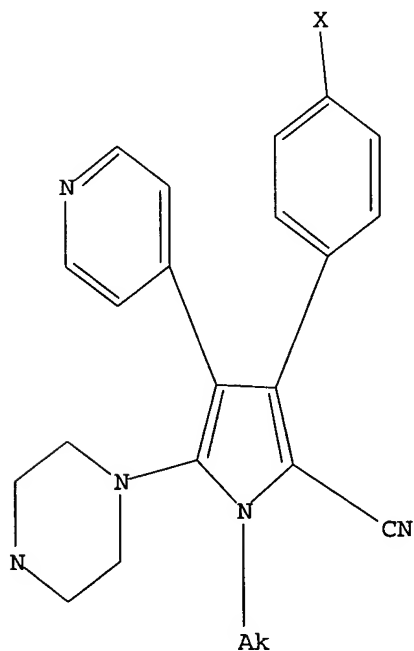
US	2006118302	08 JUN 2006
DE	102004054303	11 MAY 2006
EP	1657292	17 MAY 2006
JP	2006120460	11 MAY 2006
WO	2006053912	26 MAY 2006
GB	2419594	03 MAY 2006
FR	2877567	12 MAY 2006
RU	2275374	27 APR 2006
CA	2518664	10 MAR 2006

Expanded G-group definition display now available.

New CAS Information Use Policies, enter HELP USAGETERMS for details.

=> d stat que L34

L12 STR



Structure attributes must be viewed using STN Express query preparation.

L34 1 SEA FILE=MARPAT SSS FUL L12

100.0% PROCESSED 2804 ITERATIONS  
SEARCH TIME: 00.00.06

1 ANSWERS

=> file wpix

FILE 'WPIX' ENTERED AT 15:23:45 ON 28 JUL 2006  
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FILE LAST UPDATED: 24 JUL 2006 <20060724/UP>  
MOST RECENT DERWENT UPDATE: 200647 <200647/DW>  
DERWENT WORLD PATENTS INDEX SUBSCRIBER FILE, COVERS 1963 TO DATE

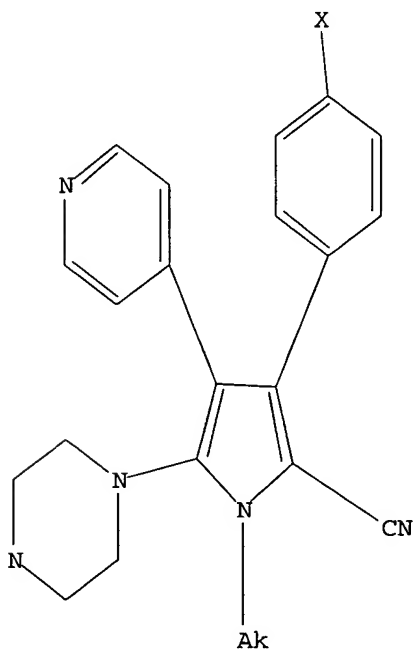
>>> FOR A COPY OF THE DERWENT WORLD PATENTS INDEX STN USER GUIDE,  
PLEASE VISIT:  
[http://www.stn-international.de/training\\_center/patents/stn\\_guide.pdf](http://www.stn-international.de/training_center/patents/stn_guide.pdf) <

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<http://scientific.thomson.com/support/patents/coverage/latestupdates/>

>>> PLEASE BE AWARE OF THE NEW IPC REFORM IN 2006, SEE  
[http://www.stn-international.de/stndatabases/details/ipc\\_reform.html](http://www.stn-international.de/stndatabases/details/ipc_reform.html) and  
<http://scientific.thomson.com/media/scpdf/ipcrdpi.pdf> <<<

>>> FOR FURTHER DETAILS ON THE FORTHCOMING DERWENT WORLD PATENTS  
INDEX ENHANCEMENTS PLEASE VISIT:  
[http://www.stn-international.de/stndatabases/details/dwpi\\_r.html](http://www.stn-international.de/stndatabases/details/dwpi_r.html) <<<  
'BIX' IS DEFAULT SEARCH FIELD FOR 'WPIX' FILE

=> d stat que L46  
L12 STR



Structure attributes must be viewed using STN Express query preparation.

L42 2 SEA FILE=WPIX SSS FUL L12  
L43 1 SEA FILE=WPIX ABB=ON PLU=ON (RADZT1/DCN OR RADZT3/DCN)  
L44 1 SEA FILE=WPIX ABB=ON PLU=ON (888697-0-0-0/DCRE OR 888700-0-0-0/DCRE)  
L45 1 SEA FILE=WPIX ABB=ON PLU=ON L42/DCR  
L46 1 SEA FILE=WPIX ABB=ON PLU=ON (L43 OR L44 OR L45)

=> dup rem L16 L32 L34 L46

L32 HAS NO ANSWERS

DUPLICATE IS NOT AVAILABLE IN 'BEILSTEIN'.

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PROCESSING COMPLETED FOR L16

PROCESSING COMPLETED FOR L32

PROCESSING COMPLETED FOR L34

PROCESSING COMPLETED FOR L46

L50 1 DUP REM L16 L32 L34 L46 (2 DUPLICATES REMOVED)

ANSWER '1' FROM FILE HCAPLUS

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L50 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 1

ACCESSION NUMBER: 2004:292020 HCAPLUS

DOCUMENT NUMBER: 140:321233

TITLE: A preparation of pyrrole derivatives useful for the treatment of disorders ameliorated by reduction of TNF- $\alpha$  production and/or p38 activity

INVENTOR(S): Bullington, James L.; Fan, Xiaodong; Jackson, Paul F.; Zhang, Yue-mei

PATENT ASSIGNEE(S): Janssen Pharmaceutica N.V., Belg.

SOURCE: PCT Int. Appl., 116 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

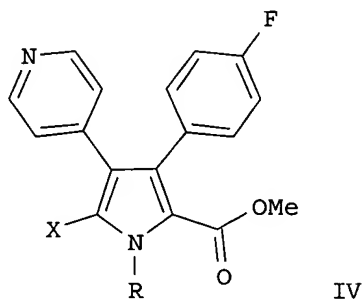
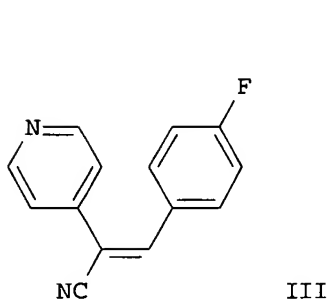
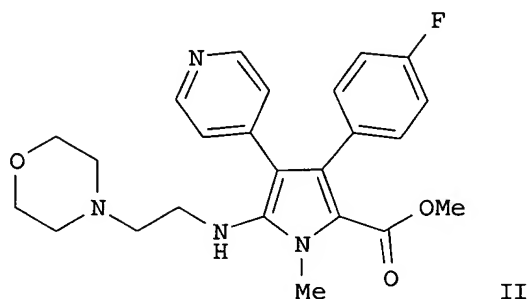
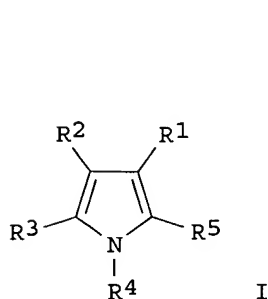
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004029040	A1	20040408	WO 2003-US30223	20030924
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES,			

FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF,  
 BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

CA 2500221	AA	20040408	CA 2003-2500221	20030924
AU 2003278927	A1	20040419	AU 2003-278927	20030924
US 2005043331	A1	20050224	US 2003-670031	20030924
EP 1549635	A1	20050706	EP 2003-770442	20030924
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BR 2003014783	A	20050726	BR 2003-14783	20030924
CN 1701069	A	20051123	CN 2003-825319	20030924
JP 2006511479	T2	20060406	JP 2004-539896	20030924
NO 2005001967	A	20050621	NO 2005-1967	20050422
PRIORITY APPLN. INFO.:			US 2002-414436P	P 20020927
			WO 2003-US30223	W 20030924
OTHER SOURCE(S):		MARPAT 140:321233		
GI				



AB The invention relates to 3-pyridyl-4-arylpyrrole derivs. of formula I [wherein: R1 and R2 are independently selected from (un)substituted (hetero)aryl; R3 = H, (un)substituted alkyl, -N:CR6-, -C(O)R7, etc.; R4 = H, (un)substituted alkyl, (un)substituted (hetero)aryl, etc.; R5 = (un)substituted alkyl, C(O)OR7, C(O)R7, CN, NO2, halo, etc.; R6 and R7 are independently selected from H, (un)substituted alkyl, (un)substituted aryl, (un)substituted heterocycle; with provisos], and pharmaceutical compns. comprising the same, useful for treating disorders ameliorated by reducing TNF- $\alpha$  production and/or p38 activity in appropriate cells. The invention compds. I were screened for p38 inhibition (in-vitro enzyme assays) and TNF- $\alpha$  inhibition (in-vitro whole cell assays and in vivo rodent assay). The invention also provides therapeutic and prophylactic methods using the instant pharmaceutical compns. For instance, pyrrole derivative II (compound 5; mouse 10 mg/kg, 0.5 h, 44% inhibition of TNF- $\alpha$



production) was prepared via condensation of 4-fluorobenzaldehyde with 4-pyridylacetonitrile, heterocyclization of the obtained pyridine derivative III with Me isocyanoacetate, N-methylation of the pyrrole ring of the obtained pyrrolicarboxylate derivative IV (X = H, R = H), bromination of the pyrrolicarboxylate derivative IV (X = H, R = Me), and subsequent amination of the obtained bromopyrrole derivative IV (X = Br, R = Me) by 4-(2-aminoethyl)morpholine.

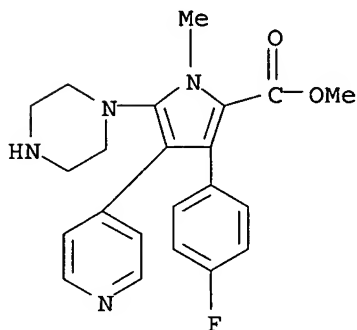
IT 678161-35-8P 678161-52-9P

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(intermediate; preparation of pyridyl(aryl)pyrrole derivs. useful for the treatment of disorders ameliorated by reduction of TNF- $\alpha$  production and/or p38 activity)

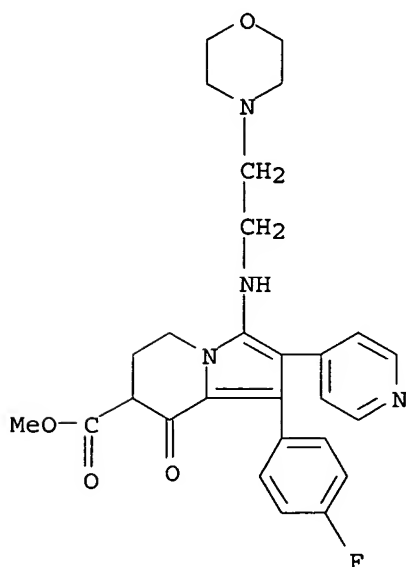
RN 678161-35-8 HCAPLUS

CN 1H-Pyrrole-2-carboxylic acid, 3-(4-fluorophenyl)-1-methyl-5-(1-piperazinyl)-4-(4-pyridinyl)-, methyl ester (9CI) (CA INDEX NAME)



RN 678161-52-9 HCAPLUS

CN 7-Indolizinecarboxylic acid, 1-(4-fluorophenyl)-5,6,7,8-tetrahydro-3-[[2-(4-morpholinyl)ethyl]amino]-8-oxo-2-(4-pyridinyl)-, methyl ester (9CI) (CA INDEX NAME)

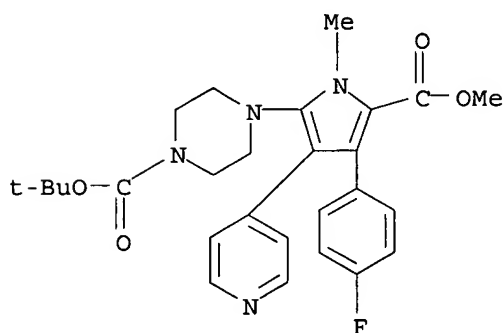


IT 678161-34-7

RL: PAC (Pharmacological activity); RCT (Reactant); THU (Therapeutic use);  
 BIOL (Biological study); RACT (Reactant or reagent); USES (Uses)  
 (preparation of pyridyl(aryl)pyrrole derivs. useful for the treatment of  
 disorders ameliorated by reduction of TNF- $\alpha$  production and/or p38  
 activity)

RN 678161-34-7 HCAPLUS

CN 1-Piperazinecarboxylic acid, 4-[4-(4-fluorophenyl)-5-(methoxycarbonyl)-1-methyl-3-(4-pyridinyl)-1H-pyrrol-2-yl]-, 1,1-dimethylethyl ester (9CI)  
 (CA INDEX NAME)



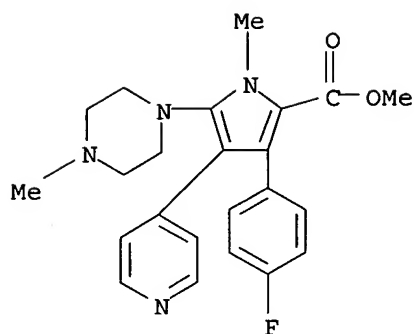
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RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU  
 (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES  
 (Uses)

(preparation of pyridyl(aryl)pyrrole derivs. useful for the treatment of  
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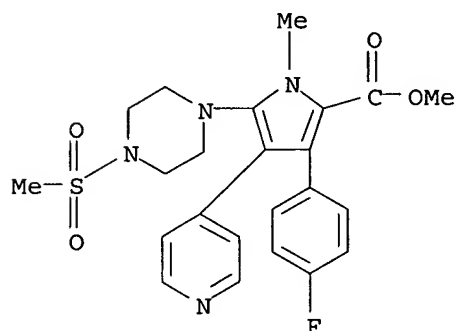
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CN 1H-Pyrrole-2-carboxylic acid, 3-(4-fluorophenyl)-1-methyl-5-(4-methyl-1-piperazinyl)-4-(4-pyridinyl)-, methyl ester (9CI) (CA INDEX NAME)



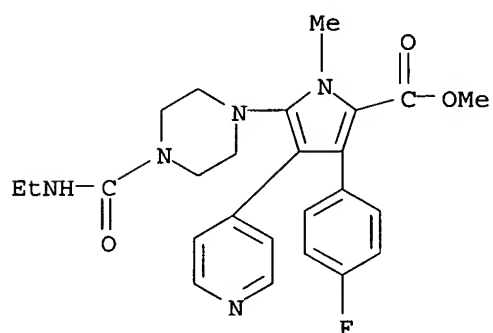
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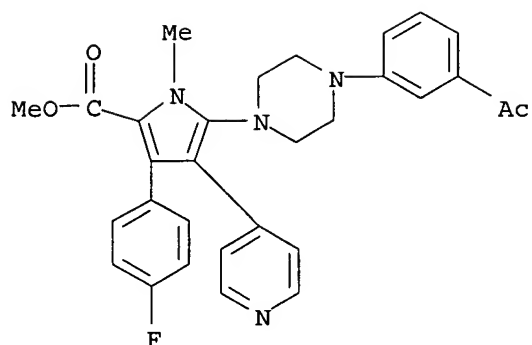
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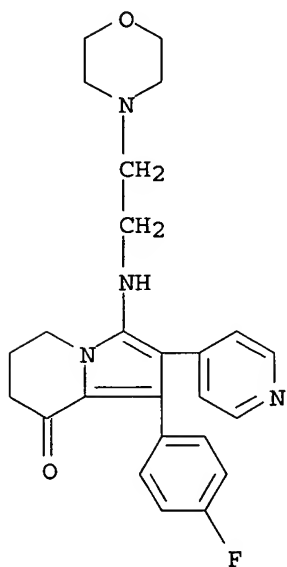
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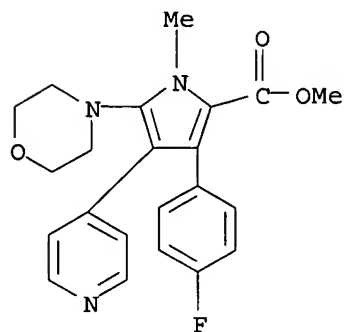
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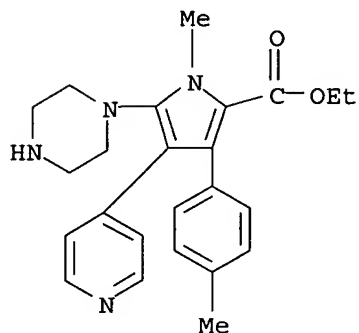


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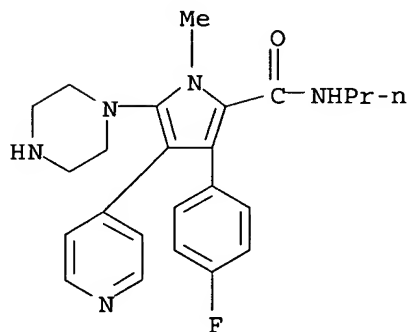
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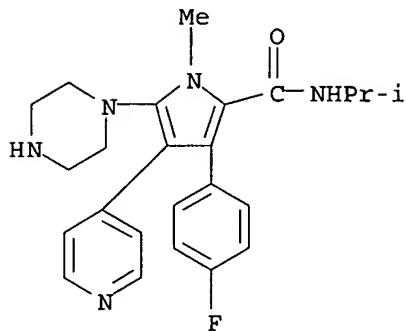
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CN 1H-Pyrrole-2-carboxylic acid, 1-methyl-3-(4-methylphenyl)-5-(1-piperazinyl)-4-(4-pyridinyl)-, ethyl ester (9CI) (CA INDEX NAME)



RN 678162-34-0 HCAPLUS  
CN 1H-Pyrrole-2-carboxamide, 3-(4-fluorophenyl)-1-methyl-5-(1-piperazinyl)-N-propyl-4-(4-pyridinyl)- (9CI) (CA INDEX NAME)

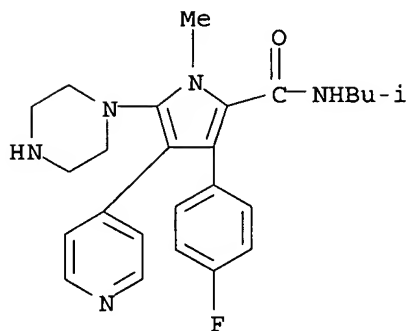


RN 678162-35-1 HCAPLUS  
CN 1H-Pyrrole-2-carboxamide, 3-(4-fluorophenyl)-1-methyl-N-(1-methylethyl)-5-(1-piperazinyl)-4-(4-pyridinyl)- (9CI) (CA INDEX NAME)



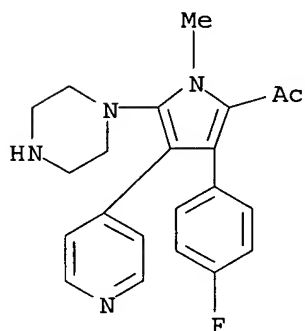
RN 678162-36-2 HCAPLUS  
CN 1H-Pyrrole-2-carboxamide, 3-(4-fluorophenyl)-1-methyl-N-(2-methylpropyl)-5-

(1-piperazinyl)-4-(4-pyridinyl)- (9CI) (CA INDEX NAME)



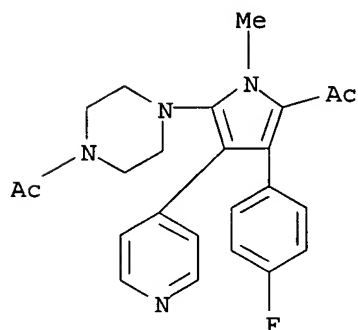
RN 678162-37-3 HCAPLUS

CN Ethanone, 1-[3-(4-fluorophenyl)-1-methyl-5-(1-piperazinyl)-4-(4-pyridinyl)-1H-pyrrol-2-yl]- (9CI) (CA INDEX NAME)



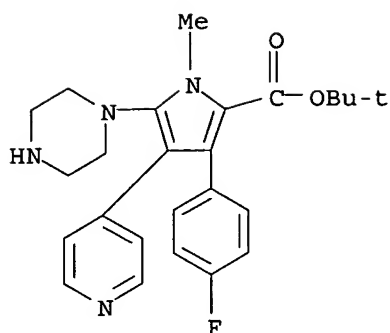
RN 678162-39-5 HCAPLUS

CN Piperazine, 1-acetyl-4-[5-acetyl-4-(4-fluorophenyl)-1-methyl-3-(4-pyridinyl)-1H-pyrrol-2-yl]- (9CI) (CA INDEX NAME)



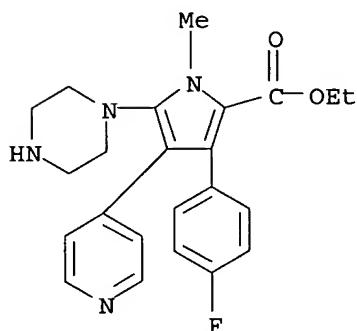
RN 678162-41-9 HCAPLUS

CN 1H-Pyrrole-2-carboxylic acid, 3-(4-fluorophenyl)-1-methyl-5-(1-piperazinyl)-4-(4-pyridinyl)-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



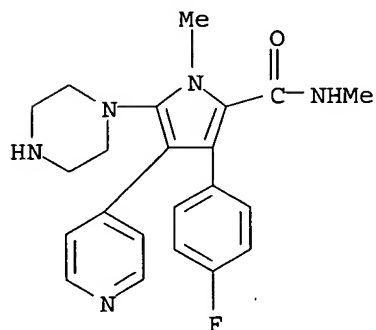
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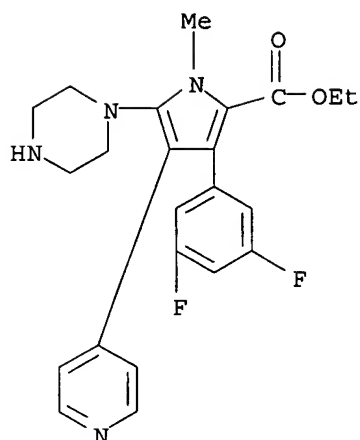
RN 678162-45-3 HCAPLUS

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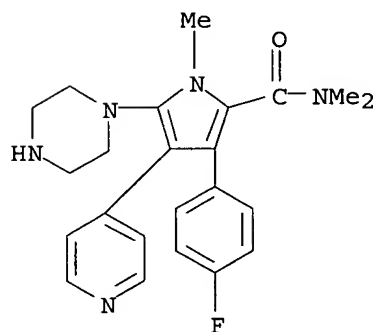
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CN 1H-Pyrrole-2-carboxylic acid, 3-(3,5-difluorophenyl)-1-methyl-5-(1-piperazinyl)-4-(4-pyridinyl)-, ethyl ester (9CI) (CA INDEX NAME)



RN 678162-47-5 HCAPLUS

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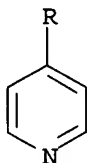
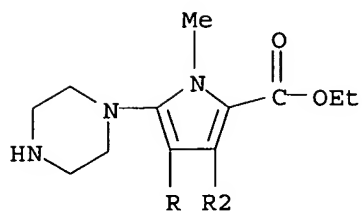


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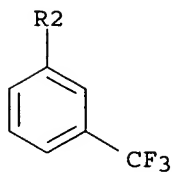
CN 1H-Pyrrole-2-carboxylic acid, 1-methyl-5-(1-piperazinyl)-4-(4-pyridinyl)-3-[3-(trifluoromethyl)phenyl]-, ethyl ester (9CI) (CA INDEX NAME)



PAGE 1-A

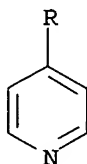
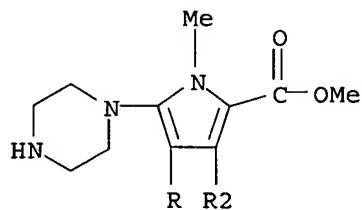


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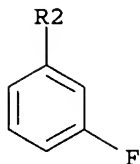


RN 678162-51-1 HCAPLUS  
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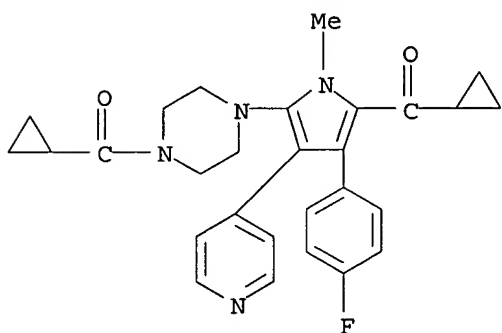
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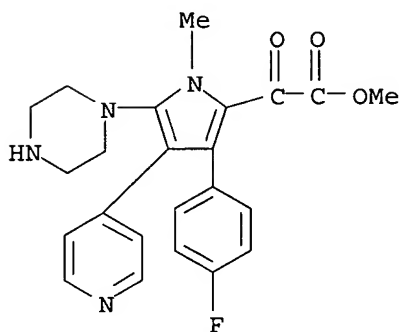
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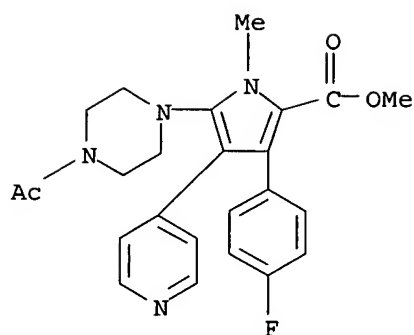
RN 678162-52-2 HCAPLUS  
 CN Piperazine, 1-(cyclopropylcarbonyl)-4-[5-(cyclopropylcarbonyl)-4-(4-fluorophenyl)-1-methyl-3-(4-pyridinyl)-1H-pyrrol-2-yl]- (9CI) (CA INDEX NAME)



RN 678162-53-3 HCAPLUS  
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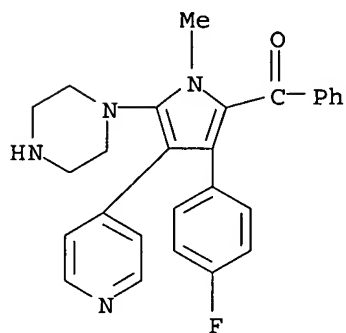


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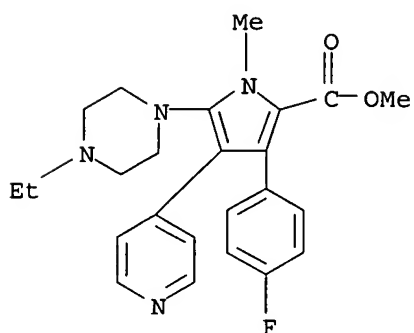
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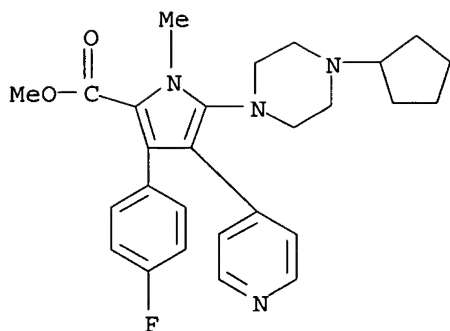
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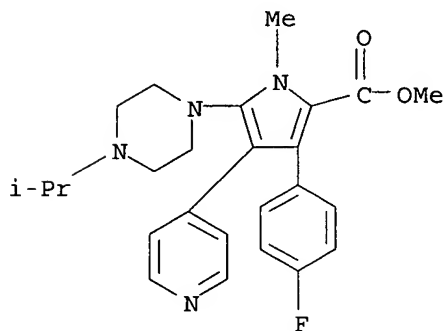
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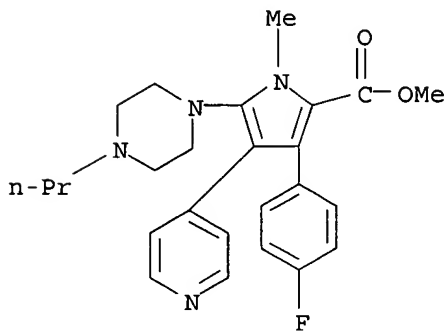
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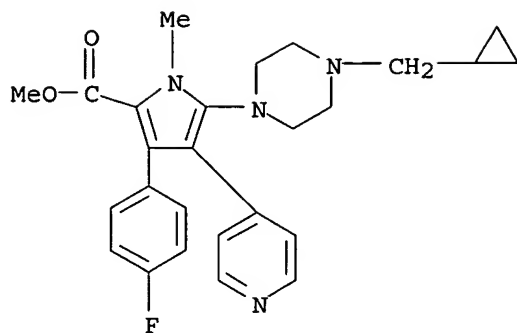
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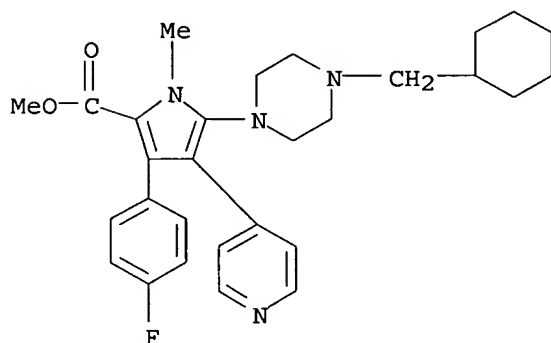
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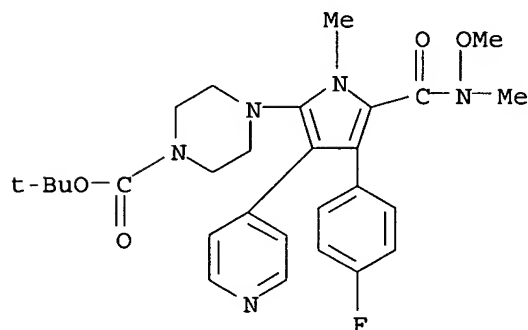
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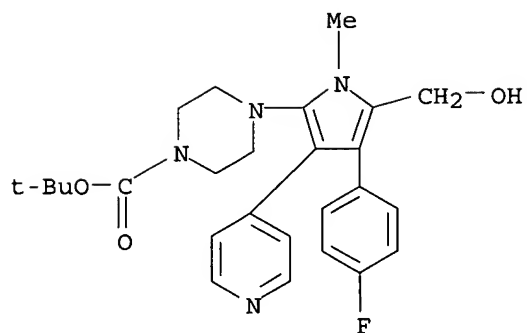
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CN 1-Piperazinecarboxylic acid, 4-[4-(4-fluorophenyl)-5-[(methoxymethylamino)carbonyl]-1-methyl-3-(4-pyridinyl)-1H-pyrrol-2-yl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



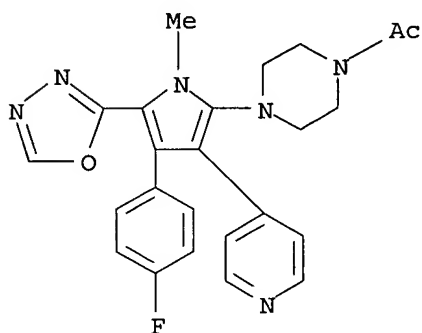
RN 678162-99-7 HCAPLUS

CN 1-Piperazinecarboxylic acid, 4-[4-(4-fluorophenyl)-5-(hydroxymethyl)-1-methyl-3-(4-pyridinyl)-1H-pyrrol-2-yl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



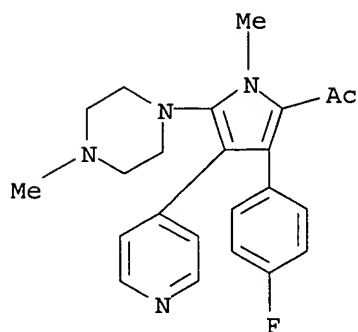
RN 678163-05-8 HCAPLUS

CN	Piperazine, 1-acetyl-4-[4-(4-fluorophenyl)-1-methyl-5-(1,3,4-oxadiazol-2-yl)-3-(4-pyridinyl)-1H-pyrrol-2-yl]- (9CI) (CA INDEX NAME)
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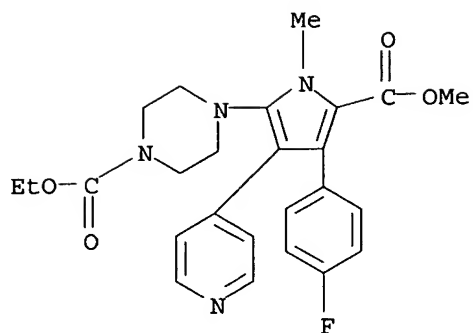
RN 678163-25-2 HCAPLUS

CN      Ethanone, 1-[3-(4-fluorophenyl)-1-methyl-5-(4-methyl-1-piperazinyl)-4-(4-pyridinyl)-1H-pyrrol-2-yl]- (9CI)      (CA INDEX NAME)



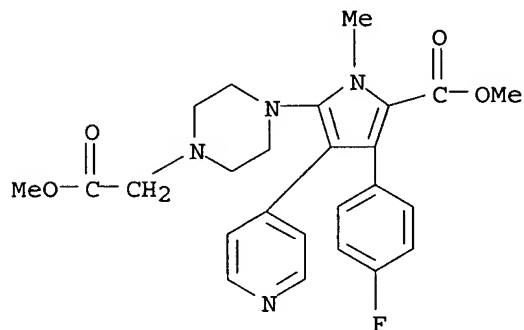
RN 678163-26-3 HCAPLUS

CN 1-Piperazinecarboxylic acid, 4-[4-(4-fluorophenyl)-5-(methoxycarbonyl)-1-methyl-3-(4-pyridinyl)-1H-pyrrol-2-yl]-, ethyl ester (9CI) (CA INDEX NAME)



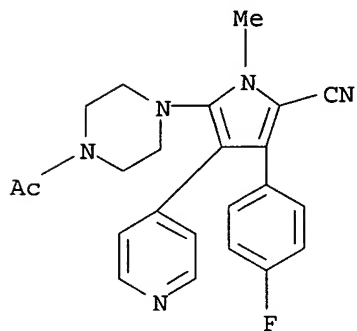
RN 678163-28-5 HCAPLUS

CN 1-Piperazineacetic acid, 4-[4-(4-fluorophenyl)-5-(methoxycarbonyl)-1-methyl-3-(4-pyridinyl)-1H-pyrrol-2-yl]-, methyl ester (9CI) (CA INDEX NAME)



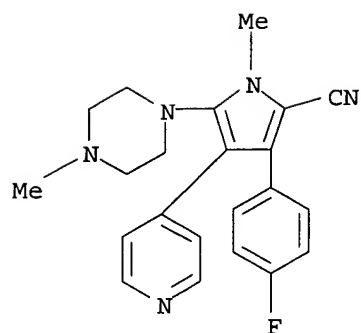
RN 678163-29-6 HCAPLUS

CN Piperazine, 1-acetyl-4-[5-cyano-4-(4-fluorophenyl)-1-methyl-3-(4-pyridinyl)-1H-pyrrol-2-yl]- (9CI) (CA INDEX NAME)



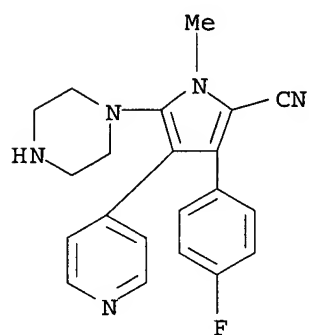
RN 678163-30-9 HCAPLUS

CN 1H-Pyrrole-2-carbonitrile, 3-(4-fluorophenyl)-1-methyl-5-(4-methyl-1-piperazinyl)-4-(4-pyridinyl)- (9CI) (CA INDEX NAME)



RN 678163-33-2 HCAPLUS

CN 1H-Pyrrole-2-carbonitrile, 3-(4-fluorophenyl)-1-methyl-5-(1-piperazinyl)-4-(4-pyridinyl)- (9CI) (CA INDEX NAME)





STRUCTURE SEARCH  
(BROAD)

=&gt; □

=&gt; file registry

FILE 'REGISTRY' ENTERED AT 15:25:46 ON 28 JUL 2006

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STRUCTURE FILE UPDATES: 27 JUL 2006 HIGHEST RN 896463-29-9

DICTIONARY FILE UPDATES: 27 JUL 2006 HIGHEST RN 896463-29-9

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 6, 2006

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experimental property data in the original document. For information  
on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

=&gt; file hcaplus

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FILE COVERS 1907 - 28 Jul 2006 VOL 145 ISS 6

FILE LAST UPDATED: 27 Jul 2006 (20060727/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate  
substance identification.

'OBI' IS DEFAULT SEARCH FIELD FOR 'HCAPLUS' FILE

=&gt; d stat que L11

L1 886180 SEA FILE=REGISTRY ABB=ON PLU=ON (NC4/ESS AND NRS&gt;2 AND N&gt;1

L3 AND (>1 Q/REL))  
STR

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

Structure attributes must be viewed using STN Express query preparation.

L5 174 SEA FILE=REGISTRY SUB=L1 SSS FUL L3

L7 STR

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

Structure attributes must be viewed using STN Express query preparation.

L9 106 SEA FILE=REGISTRY SUB=L5 SSS FUL L7

L10 68 SEA FILE=REGISTRY ABB=ON PLU=ON L5 NOT L9

L11 8 SEA FILE=HCAPLUS ABB=ON PLU=ON L10

=> => s L11 not L16

L52 7 L11 NOT L16

*narrow structure search*

=> d ibib abs hitstr L52 1-7

L52 ANSWER 1 OF 7 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2001:559491 HCAPLUS

DOCUMENT NUMBER: 135:137517

TITLE: Preparation of pyridyl- and pyrimidinyl-substituted fused pyrroles as cytokine inhibitors

INVENTOR(S): Striegel, Hans-Guenter; Laufer, Stefan; Tollmann Neher, Karola; Tries, Susanne

PATENT ASSIGNEE(S): Merckle GmbH Chemisch Pharmazeutische Fabrik, Germany

SOURCE: Ger. Offen., 22 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent

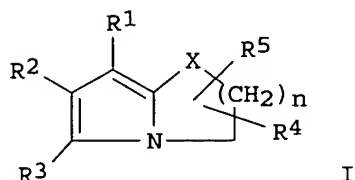
LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 10004157	A1	20010802	DE 2000-10004157	20000201
CA 2398111	AA	20010809	CA 2001-2398111	20010131
WO 2001057042	A2	20010809	WO 2001-EP1011	20010131
WO 2001057042	A3	20011227		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
EP 1252163	A2	20021030	EP 2001-902370	20010131
EP 1252163	B1	20030924		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2003525227	T2	20030826	JP 2001-557873	20010131
AT 250608	E	20031015	AT 2001-902370	20010131
PT 1252163	T	20040227	PT 2001-902370	20010131
ES 2208548	T3	20040616	ES 2001-1902370	20010131

NO 2002003634 A 20020925 NO 2002-3634 20020731  
 US 2003153558 A1 20030814 US 2002-182579 20021105  
 US 6867211 B2 20050315  
 PRIORITY APPLN. INFO.: DE 2000-10004157 A 20000201  
 WO 2001-EP1011 W 20010131  
 OTHER SOURCE(S): CASREACT 135:137517; MARPAT 135:137517  
 GI



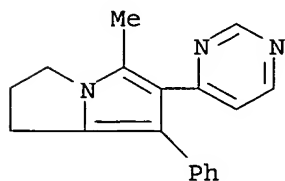
AB Title compds. [I; the first of R1-R3 = (substituted) 4-pyridyl, 2,4-pyrimidyl, 3-amino-2,4-pyrimidinyl; the second of R1-R3 = (substituted) Ph, thienyl; the third of R1-R3 = H, CO<sub>2</sub>H, alkoxycarbonyl, CH<sub>2</sub>OH, alkyl; R4, R5 = H, alkyl; X = CH<sub>2</sub>, S, O; n = 1, 2], and their use as pharmaceuticals is claimed. Thus, 3-(4-fluorophenyl)-2-(4-pyridyl)-5,6,7,8-tetrahydroindolizine-1-carboxylic acid Et ester (preparation given) in THF was treated dropwise at room temperature with NaAlH<sub>2</sub>(OCH<sub>2</sub>CH<sub>2</sub>OMe)<sub>2</sub> in PhMe followed by stirring for 24 h at 40° to give 95% [3-(4-fluorophenyl)-2-(4-pyridyl)-5,6,7,8-tetrahydroindolizine-1-yl]methanol. Several I inhibited tumor necrosis factor (TNFα), interleukin (IL-1β), 5-lipoxygenase, cyclooxygenase-1, and cyclooxygenase-2 with IC<sub>50</sub> = 0.027-100 μmol.

IT 351493-39-5P 351493-40-8P 351493-42-0P  
 351493-43-1P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (preparation of pyridyl- and pyrimidinyl-substituted fused pyrroles as cytokine inhibitors)

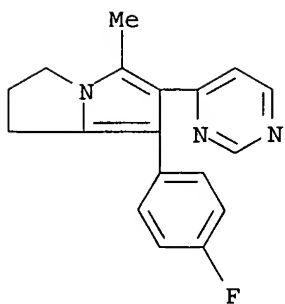
RN 351493-39-5 HCAPLUS

CN 1H-Pyrrolizine, 2,3-dihydro-5-methyl-7-phenyl-6-(4-pyrimidinyl) - (9CI)  
 (CA INDEX NAME)

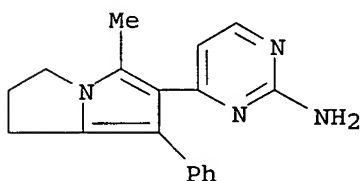


RN 351493-40-8 HCAPLUS

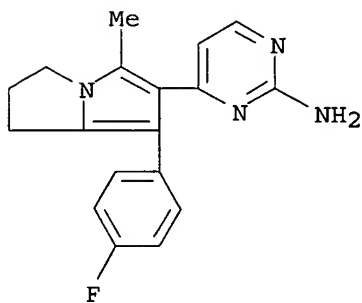
CN 1H-Pyrrolizine, 7-(4-fluorophenyl)-2,3-dihydro-5-methyl-6-(4-pyrimidinyl) - (9CI) (CA INDEX NAME)



RN 351493-42-0 HCAPLUS  
CN 2-Pyrimidinamine, 4-(2,3-dihydro-5-methyl-7-phenyl-1H-pyrrolizin-6-yl)-  
(9CI) (CA INDEX NAME)



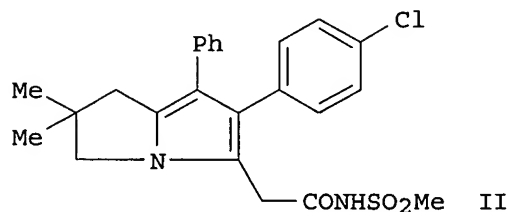
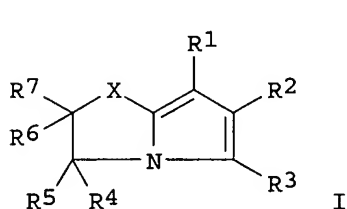
RN 351493-43-1 HCAPLUS  
CN 2-Pyrimidinamine, 4-[7-(4-fluorophenyl)-2,3-dihydro-5-methyl-1H-pyrrolizin-  
6-yl]- (9CI) (CA INDEX NAME)



L52 ANSWER 2 OF 7 HCAPLUS COPYRIGHT 2006 ACS on STN  
ACCESSION NUMBER: 1996:155517 HCAPLUS  
DOCUMENT NUMBER: 124:202010  
TITLE: Preparation of N-sulfonylpyrrolizineacetamides and  
analogs as cyclooxygenase and lipooxygenase inhibitors  
INVENTOR(S): Laufer, Stefan; Striegel, Hans Guenther; Dannhardt,  
Gerd  
PATENT ASSIGNEE(S): Merckle GmbH, Germany  
SOURCE: Ger. Offen., 22 pp.  
CODEN: GWXXBX  
DOCUMENT TYPE: Patent  
LANGUAGE: German  
FAMILY ACC. NUM. COUNT: 1

## PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 4419247	A1	19951207	DE 1994-4419247	19940601
CA 2191746	AA	19951207	CA 1995-2191746	19950531
WO 9532972	A1	19951207	WO 1995-EP2079	19950531
W: AM, AU, BB, BG, BR, BY, CA, CN, CZ, EE, FI, GE, HU, IS, JP, KG, KP, KR, KZ, LK, LR, LT, LV, MD, MG, MN, MX, NO, NZ, PL, RO, RU, SG, SI, SK, TJ, TT, UA, US, UZ, VN				
RW: KE, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AU 9526730	A1	19951221	AU 1995-26730	19950531
EP 763037	A1	19970319	EP 1995-921801	19950531
EP 763037	B1	20011114		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
JP 10506370	T2	19980623	JP 1996-500334	19950531
JP 3671303	B2	20050713		
AT 208777	E	20011115	AT 1995-921801	19950531
ES 2166823	T3	20020501	ES 1995-921801	19950531
PT 763037	T	20020531	PT 1995-921801	19950531
NO 9605095	A	19961129	NO 1996-5095	19961129
NO 310076	B1	20010514		
FI 9604773	A	19970127	FI 1996-4773	19961129
FI 114099	B1	20040813		
US 5942535	A	19990824	US 1997-737921	19970328
PRIORITY APPLN. INFO.:			DE 1994-4419247	A 19940601
OTHER SOURCE(S):			WO 1995-EP2079	W 19950531
GI			MARPAT 124:202010	



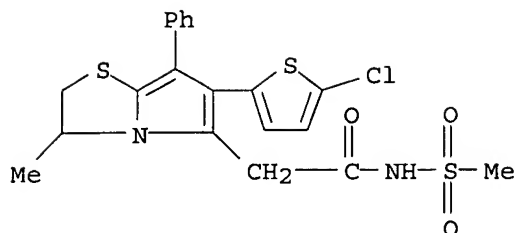
AB Title compds. [I; 2 of R1-R3 = H or (hetero)aryl and the other = COCO2H, alkoxy carbonyl, sulfonyl carbamoyl alkyl, etc.; R4-R7 = H or alkyl; 2 vicinal R4-R7 = bond; X = CH2, O, S, (alkyl)imino, etc] were prepared Thus, title compound II had IC50 of 2.3x10<sup>-7</sup> and 1.5x10<sup>-7</sup> (units not given) against lipoxigenase and cyclooxygenase, resp.

IT 174348-04-0P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(preparation of N-sulfonylpyrrolizineacetamides and analogs as cyclooxygenase and lipoxigenase inhibitors)

RN 174348-04-0 HCAPLUS

CN Pyrrolo[2,1-b]thiazole-5-acetamide, 6-(5-chloro-2-thienyl)-2,3-dihydro-3-methyl-N-(methylsulfonyl)-7-phenyl- (9CI) (CA INDEX NAME)



L52 ANSWER 3 OF 7 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1996:155516 HCAPLUS

DOCUMENT NUMBER: 124:202009

TITLE: Preparation of heteroarylpyrrolizineacetates and  
analogs as cyclooxygenase and lipooxygenase inhibitors  
INVENTOR(S): Laufer, Stefan; Striegel, Hans Guenther; Dannhardt,  
Gerd

PATENT ASSIGNEE(S): Merckle GmbH, Germany

SOURCE: Ger. Offen., 25 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 4419246	A1	19951207	DE 1994-4419246	19940601
CA 2191747	AA	19951207	CA 1995-2191747	19950531
WO 9532970	A1	19951207	WO 1995-EP2077	19950531
W: AM, AU, BB, BG, BR, BY, CA, CN, CZ, EE, FI, GE, HU, IS, JP, KG, KP, KR, KZ, LK, LR, LT, LV, MD, MG, MN, MX, NO, NZ, PL, RO, RU, SG, SI, SK, TJ, TT, UA, US, UZ, VN				
RW: KE, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AU 9526728	A1	19951221	AU 1995-26728	19950531
EP 763036	A1	19970319	EP 1995-921799	19950531
EP 763036	B1	20020911		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
JP 10506368	T2	19980623	JP 1996-500332	19950531
JP 3671302	B2	20050713		
AT 223917	E	20020915	AT 1995-921799	19950531
PT 763036	T	20021231	PT 1995-921799	19950531
ES 2182903	T3	20030316	ES 1995-921799	19950531
US 5958943	A	19990928	US 1996-737919	19960328
NO 9605093	A	19961129	NO 1996-5093	19961129
NO 310291	B1	20010618		
FI 9604771	A	19970127	FI 1996-4771	19961129
FI 113964	B1	20040715		

PRIORITY APPLN. INFO.:

DE 1994-4419246

A 19940601

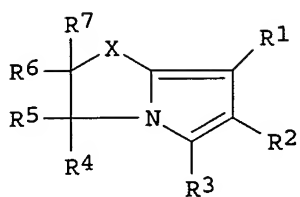
WO 1995-EP2077

W 19950531

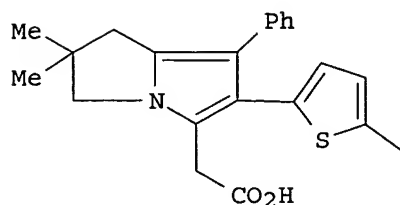
OTHER SOURCE(S):

MARPAT 124:202009

GI



I



II

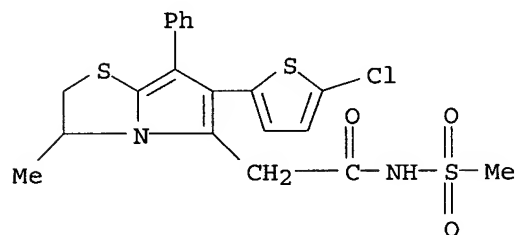
AB Title compds. [I; 1 of R1-R3 = heteroaryl, 1 of the remaining = H or (hetero)aryl, and the remaining = H, CHO, carboxy(alkyl), alkoxy(alkyl), etc.; R4-R7 = H or alkyl; 2 of vicinal R4-R7 = bond; X = CH<sub>2</sub>, CO, O, S, etc.] were prepared. Thus, title compound II had IC<sub>50</sub> of 4x10<sup>-7</sup> and 2x10<sup>-7</sup> (units not given) against lipoxygenase and cyclooxygenase, resp.

IT 174348-04-0P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(preparation of heteroarylpyrrolizineacetates and analogs as cyclooxygenase and lipoxygenase inhibitors)

RN 174348-04-0 HCAPLUS

CN Pyrrolo[2,1-b]thiazole-5-acetamide, 6-(5-chloro-2-thienyl)-2,3-dihydro-3-methyl-N-(methylsulfonyl)-7-phenyl- (9CI) (CA INDEX NAME)



L52 ANSWER 4 OF 7 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1982:21285 HCAPLUS

DOCUMENT NUMBER: 96:21285

TITLE: Lactone compounds containing an indolizine radical

INVENTOR(S): Becker, William J.; Farber, Sheldon; Hoover, Troy E.

PATENT ASSIGNEE(S): Appleton Papers, Inc., USA

SOURCE: U.S., 15 pp. Cont.-in-part of U.S. 4,232,887.

CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

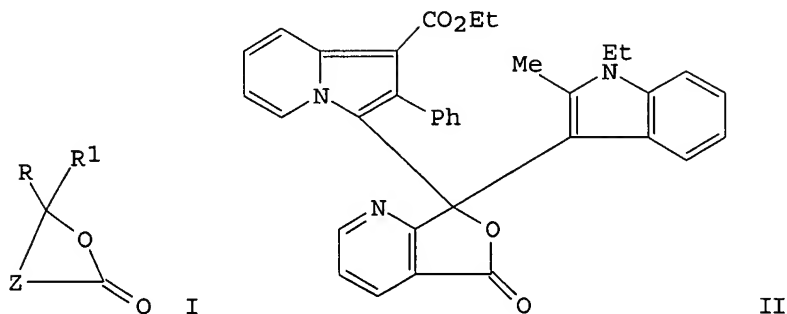
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4275206	A	19810623	US 1980-112500	19800116
US 4232887	A	19801111	US 1979-17764	19790305
CA 1147728	A1	19830607	CA 1980-345510	19800212
SE 8001604	A	19800906	SE 1980-1604	19800229
SE 454696	B	19880524		
SE 454696	C	19880901		
FI 8000652	A	19800906	FI 1980-652	19800303

FI 70035	B	19860131		
FI 70035	C	19860912		
BR 8001263	A	19801104	BR 1980-1263	19800303
BE 882057	A1	19800904	BE 1980-199656	19800304
DK 8000913	A	19800906	DK 1980-913	19800304
NO 8000611	A	19800908	NO 1980-611	19800304
ZA 8001238	A	19810325	ZA 1980-1238	19800304
ES 489160	A1	19810401	ES 1980-489160	19800304
AT 8001193	A	19840915	AT 1980-1193	19800304
AT 377761	B	19850425		
CH 656138	A	19860613	CH 1980-1714	19800304
NL 8001316	A	19800909	NL 1980-1316	19800305
NL 174146	B	19831201		
NL 174146	C	19840501		
AU 8056161	A1	19800911	AU 1980-56161	19800305
AU 540061	B2	19841101		
DE 3008475	A1	19800918	DE 1980-3008475	19800305
DE 3008475	C2	19880526		
FR 2450858	A1	19801003	FR 1980-4999	19800305
FR 2450858	B1	19811016		
GB 2044284	A	19801015	GB 1980-7564	19800305
GB 2044284	B2	19830420		
JP 55144054	A2	19801110	JP 1980-27848	19800305
JP 59044323	B4	19841029		
US 4334072	A	19820608	US 1980-192152	19800929
AT 8401458	A	19861215	AT 1984-1458	19840503
AT 383544	B	19870710		

PRIORITY APPLN. INFO.:

US 1979-17764	A2	19790305
US 1980-112500	A	19800116
AT 1980-1193	A	19800304

OTHER SOURCE(S): MARPAT 96:21285  
GI

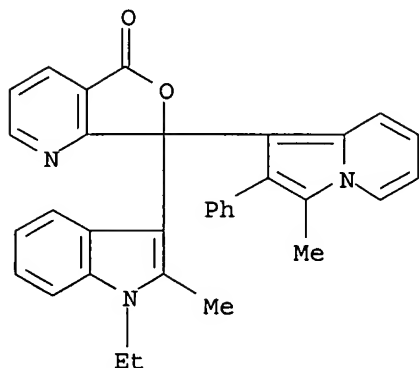
AB Chromogenic compds. (I) for pressure- or heat-sensitive mark-forming record systems are prepared, where Z = pyridine-2,3-diyl, R = substituted or unsubstituted p-aminophenyl, indol-3-yl, or 1-carbethoxy-2-phenylindolizin-3-yl (Q), and R1 = Q. I give red to green colors when in contact with acidic substrates. Thus, condensation of 3-carboxy-1-pyridinyl-1-ethyl-2-methylindol-3-yl ketone [69898-42-6] with 1-carboethoxy-2-phenylindolizine [39203-59-3] in Ac<sub>2</sub>O gave crystalline II [76949-97-8], which produced a blue color when applied to a record sheet material coated with Zn-modified phenolic resin. Numerous other chromogenic compds. were similarly prepared

IT 76949-85-4P 76949-86-5P 76949-94-5P  
76963-56-9P

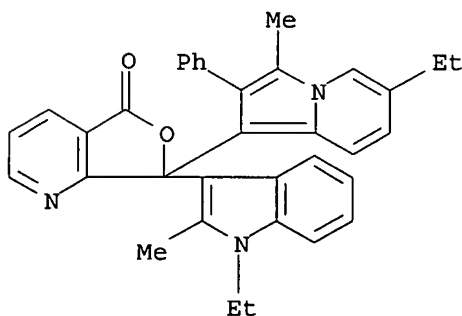


RN 76949-85-4 HCAPLUS

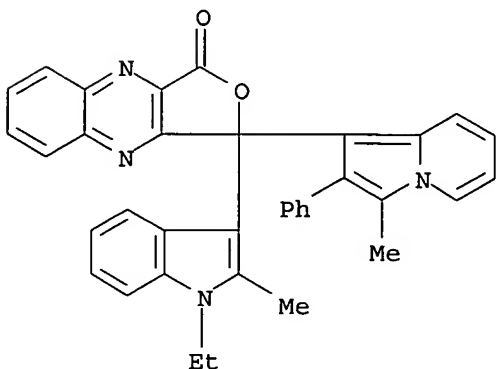
CN Furo[3,4-b]pyridin-5(7H)-one, 7-(1-ethyl-2-methyl-1H-indol-3-yl)-7-(3-methyl-2-phenyl-1-indolizinyl)- (9CI) (CA INDEX NAME)



CN Furo[3,4-b]pyridin-5(7H)-one, 7-(1-ethyl-2-methyl-1H-indol-3-yl)-7-(6-ethyl-3-methyl-2-phenyl-1-indolizinyl)- (9CI) (CA INDEX NAME)

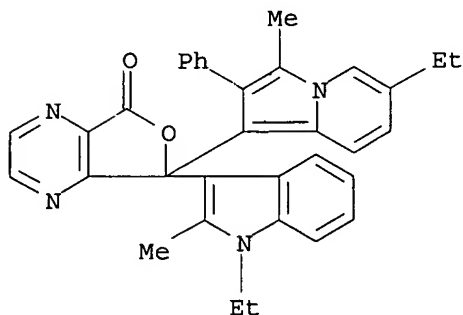


CN Furo[3,4-b]quinoxalin-1(3H)-one, 3-(1-ethyl-2-methyl-1H-indol-3-yl)-3-(3-methyl-2-phenyl-1-indoliziny)- (9CI) (CA INDEX NAME)



RN 76963-56-9 HCAPLUS

CN Furo[3,4-b]pyrazin-5(7H)-one, 7-(1-ethyl-2-methyl-1H-indol-3-yl)-7-(6-ethyl-3-methyl-2-phenyl-1-indoliziny)- (9CI) (CA INDEX NAME)



L52 ANSWER 5 OF 7 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1981:463688 HCAPLUS

DOCUMENT NUMBER: 95:63688

TITLE: Chromogenic lactone compounds and their use in pressure-sensitive and thermosensitive recording materials

INVENTOR(S): Hoover, Troy Eugene; Farber, Sheldon; Becker, William Joseph

PATENT ASSIGNEE(S): Appleton Papers, Inc., USA

SOURCE: Ger. Offen., 98 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent

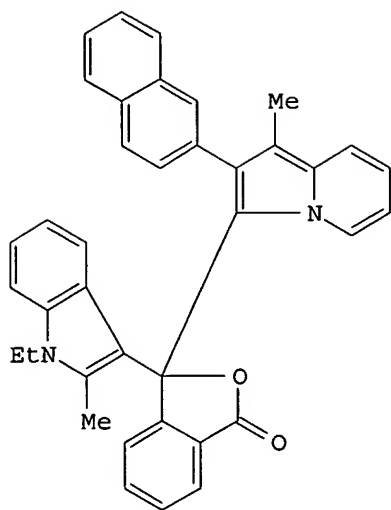
LANGUAGE: German

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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DE 3008475	A1	19800918	DE 1980-3008475	19800305
DE 3008475	C2	19880526		
US 4232887	A	19801111	US 1979-17764	19790305
US 4275206	A	19810623	US 1980-112500	19800116
PRIORITY APPLN. INFO.:			US 1979-17764	A 19790305
			US 1980-112500	A 19800116

GI



AB Chromogenic lactones containing an indolizinyll residue are prepared and used in pressure-sensitive recording materials, giving blue to green shades. Thus, a mixture of 1-ethyl-2-methylindol-3-yl 2-carboxyphenyl ketone [51389-84-5], 1-methyl-2-(2-naphthyl)indolizine [76949-58-1], and Ac<sub>2</sub>O was heated at 39° for 2 h to give I [76950-22-6], blue on a recording sheet coated with zinc-modified phenolic resin. Many similar lactones were prepared

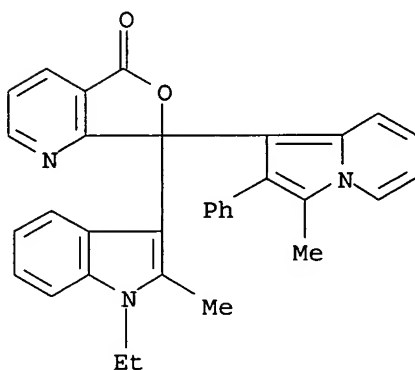
IT 76949-85-4 76949-86-5 76949-94-5  
76950-17-9 76963-56-9 77011-33-7

RL: USES (Uses)

(color formers, for copying paper, manufacture of)

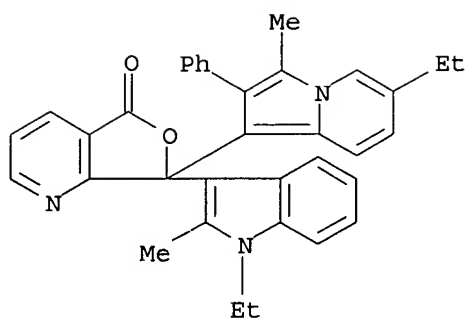
RN 76949-85-4 HCAPLUS

CN Furo[3,4-b]pyridin-5(7H)-one, 7-(1-ethyl-2-methyl-1H-indol-3-yl)-7-(3-methyl-2-phenyl-1-indolizinyll)- (9CI) (CA INDEX NAME)



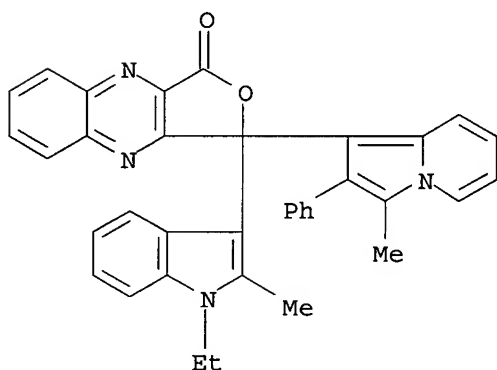
RN 76949-86-5 HCAPLUS

CN Furo[3,4-b]pyridin-5(7H)-one, 7-(1-ethyl-2-methyl-1H-indol-3-yl)-7-(6-ethyl-3-methyl-2-phenyl-1-indolizinyll)- (9CI) (CA INDEX NAME)



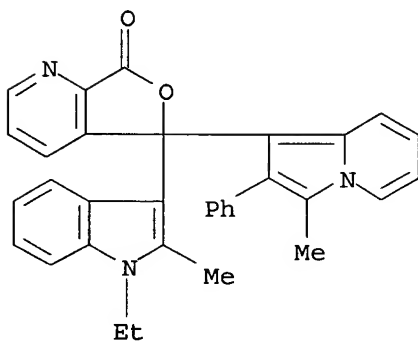
RN 76949-94-5 HCAPLUS

CN Furo[3,4-b]quinoxalin-1(3H)-one, 3-(1-ethyl-2-methyl-1H-indol-3-yl)-3-(3-methyl-2-phenyl-1-indolizinyl)- (9CI) (CA INDEX NAME)



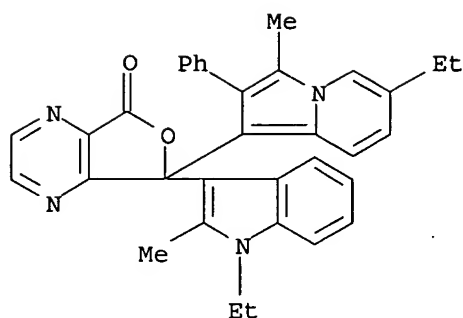
RN 76950-17-9 HCAPLUS

CN Furo[3,4-b]pyridin-7(5H)-one, 5-(1-ethyl-2-methyl-1H-indol-3-yl)-5-(3-methyl-2-phenyl-1-indolizinyl)- (9CI) (CA INDEX NAME)



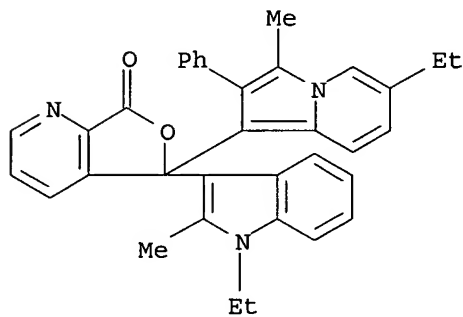
RN 76963-56-9 HCAPLUS

CN Furo[3,4-b]pyrazin-5(7H)-one, 7-(1-ethyl-2-methyl-1H-indol-3-yl)-7-(6-ethyl-3-methyl-2-phenyl-1-indolizinyl)- (9CI) (CA INDEX NAME)



RN 77011-33-7 HCAPLUS

CN Furo[3,4-b]pyridin-7(5H)-one, 5-(1-ethyl-2-methyl-1H-indol-3-yl)-5-(6-ethyl-3-methyl-2-phenyl-1-indoliziny)- (9CI) (CA INDEX NAME)



L52 ANSWER 6 OF 7 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1981:425057 HCAPLUS

DOCUMENT NUMBER: 95:25057

TITLE: Chromogenic lactone compounds and their use in pressure-sensitive and thermosensitive recording materials

INVENTOR(S): Hoover, Troy Eugene; Farber, Sheldon; Becker, William Joseph

PATENT ASSIGNEE(S): Appleton Papers, Inc., USA

SOURCE: Ger. Offen., 67 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent

LANGUAGE: German

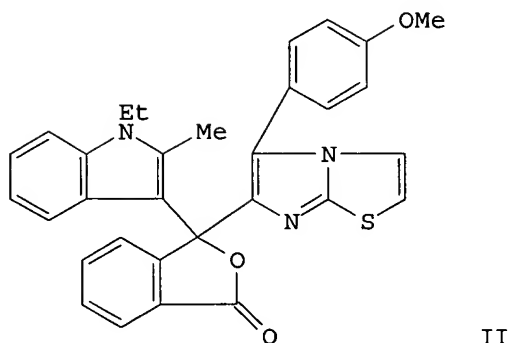
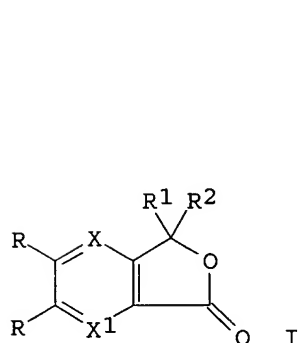
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 3008494	A1	19800918	DE 1980-3008494	19800305
DE 3008494	C2	19890406		
US 4242513	A	19801230	US 1979-17765	19790305
CA 1129855	A1	19820817	CA 1980-345054	19800205
SE 8001605	A	19800906	SE 1980-1605	19800229
SE 454274	B	19880418		
SE 454274	C	19880728		
FI 8000653	A	19800906	FI 1980-653	19800303
FI 69635	B	19851129		

FI 69635	C	19860310		
BR 8001247	A	19801104	BR 1980-1247	19800303
BE 882056	A1	19800904	BE 1980-199655	19800304
DK 8000912	A	19800906	DK 1980-912	19800304
NO 8000610	A	19800908	NO 1980-610	19800304
ZA 8001239	A	19810325	ZA 1980-1239	19800304
ES 489164	A1	19810401	ES 1980-489164	19800304
CH 656137	A	19860613	CH 1980-1713	19800304
AT 8001192	A	19880315	AT 1980-1192	19800304
AT 386833	B	19881025		
NL 8001317	A	19800909	NL 1980-1317	19800305
NL 174737	B	19840301		
NL 174737	C	19840801		
AU 8056162	A1	19800911	AU 1980-56162	19800305
AU 539167	B2	19840913		
FR 2450857	A1	19801003	FR 1980-4934	19800305
FR 2450857	B1	19811030		
GB 2044285	A	19801015	GB 1980-7565	19800305
GB 2044285	B2	19830420		
JP 55139455	A2	19801031	JP 1980-27847	19800305
JP 63020868	B4	19880430		
JP 58164642	A2	19830929	JP 1982-212045	19821202
JP 02048028	B4	19901023		
PRIORITY APPLN. INFO.:			US 1979-17765	A 19790305
			JP 1980-27847	19800305

GI



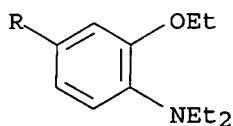
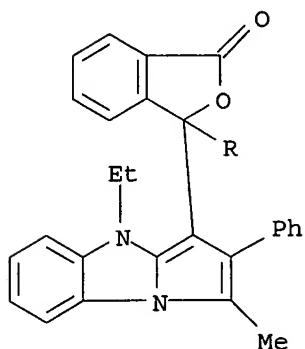
AB One hundred eleven chromogenic lactones I [R = H or RR = (CH:CH)<sub>2</sub> (RR, R<sup>1</sup> or R<sup>2</sup> may be substituted); R<sup>1</sup> = p-aminophenyl or benzimidazol-3-yl; R<sup>2</sup> = a heterocyclic moiety comprised of 2 fused aromatic rings containing a N atom in a condensation-reactive position; X = X<sup>1</sup> = CH or N, or X = N, X<sup>1</sup> = CH] were prepared, which could be encapsulated to form pressure- and thermo-sensitive copying materials which could be activated by acidic clays or resins to provide uniform light-stable coloration. Thus, 1.23 g 6-(p-methoxyphenyl)imidazo[2,1-b]thiazole heated 3 h at 50-5° with 0.92 g 2-[(1-ethyl-2-methylindol-3-yl)carbonyl]benzoic acid in 30 mL Ac<sub>2</sub>O gave 2.1 g II, which provided, with acid clay, a purple recording material.

IT 76818-29-6P 76818-34-3P 76818-40-1P  
 76818-46-7P 76818-52-5P 76818-56-9P  
 76818-59-2P 76818-62-7P 76818-65-0P  
 76818-87-6P 76823-53-5P 76840-24-9P  
 76840-38-5P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation and chromogenic property of)

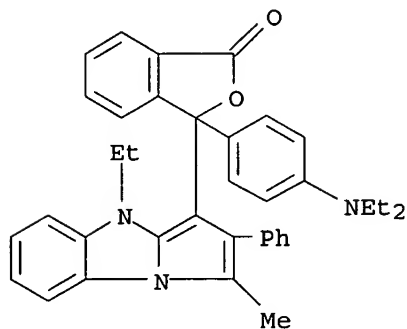
RN 76818-29-6 HCAPLUS

CN 1(3H)-Isobenzofuranone, 3-[4-(diethylamino)-3-ethoxyphenyl]-3-(4-ethyl-1-methyl-2-phenyl-4H-pyrrolo[1,2-a]benzimidazol-3-yl)- (9CI) (CA INDEX NAME)



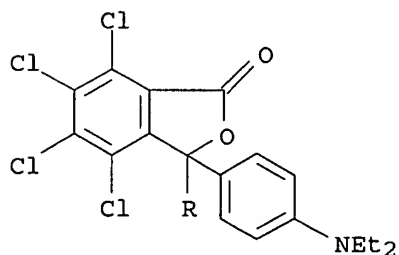
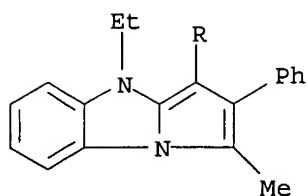
RN 76818-34-3 HCAPLUS

CN 1(3H)-Isobenzofuranone, 3-[4-(diethylamino)phenyl]-3-(4-ethyl-1-methyl-2-phenyl-4H-pyrrolo[1,2-a]benzimidazol-3-yl)- (9CI) (CA INDEX NAME)



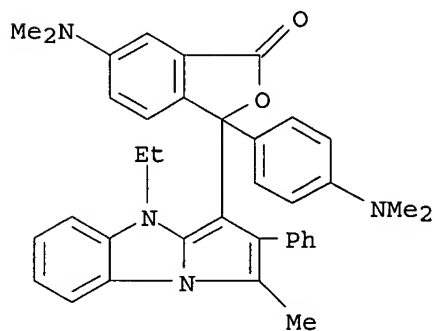
RN 76818-40-1 HCAPLUS

CN 1(3H)-Isobenzofuranone, 4,5,6,7-tetrachloro-3-[4-(diethylamino)phenyl]-3-(4-ethyl-1-methyl-2-phenyl-4H-pyrrolo[1,2-a]benzimidazol-3-yl)- (9CI) (CA INDEX NAME)



RN 76818-46-7 HCAPLUS

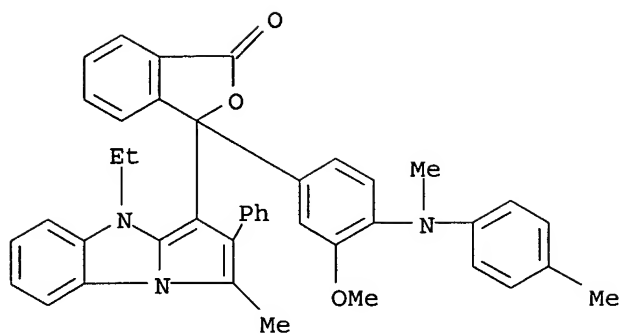
CN 1(3H)-Isobenzofuranone, 6-(dimethylamino)-3-[4-(dimethylamino)phenyl]-3-(4-ethyl-1-methyl-2-phenyl-4H-pyrrolo[1,2-a]benzimidazol-3-yl)- (9CI) (CA INDEX NAME)



RN 76818-52-5 HCAPLUS

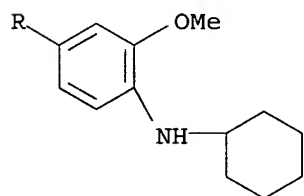
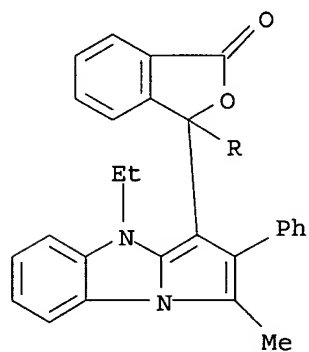
CN 1(3H)-Isobenzofuranone, 3-(4-ethyl-1-methyl-2-phenyl-4H-pyrrolo[1,2-a]benzimidazol-3-yl)-3-[3-methoxy-4-[methyl(4-methylphenyl)amino]phenyl]- (9CI) (CA INDEX NAME)





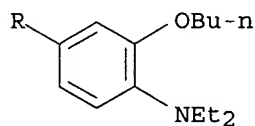
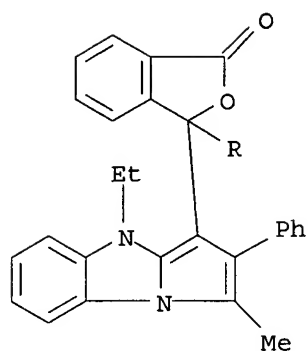
RN 76818-56-9 HCAPLUS

CN 1(3H)-Isobenzofuranone, 3-[4-(cyclohexylamino)-3-methoxyphenyl]-3-(4-ethyl-1-methyl-2-phenyl-4H-pyrrolo[1,2-a]benzimidazol-3-yl)- (9CI) (CA INDEX NAME)

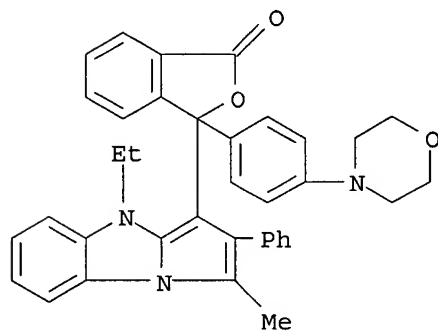


RN 76818-59-2 HCAPLUS

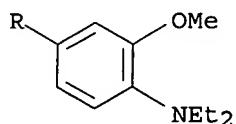
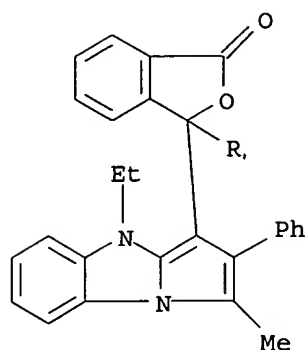
CN 1(3H)-Isobenzofuranone, 3-[3-butoxy-4-(diethylamino)phenyl]-3-(4-ethyl-1-methyl-2-phenyl-4H-pyrrolo[1,2-a]benzimidazol-3-yl)- (9CI) (CA INDEX NAME)



RN 76818-62-7 HCAPLUS  
 CN 1(3H)-Isobenzofuranone, 3-(4-ethyl-1-methyl-2-phenyl-4H-pyrrolo[1,2-a]benzimidazol-3-yl)-3-[4-(4-morpholinyl)phenyl]- (9CI) (CA INDEX NAME)



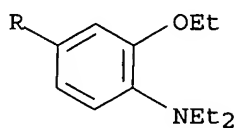
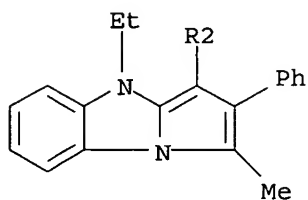
RN 76818-65-0 HCAPLUS  
 CN 1(3H)-Isobenzofuranone, 3-[4-(diethylamino)-3-methoxyphenyl]-3-(4-ethyl-1-methyl-2-phenyl-4H-pyrrolo[1,2-a]benzimidazol-3-yl)- (9CI) (CA INDEX NAME)



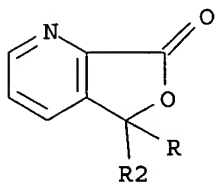
RN 76818-87-6 HCAPLUS

CN Furo[3,4-b]pyridin-7(5H)-one, 5-[4-(diethylamino)-3-ethoxyphenyl]-5-(4-ethyl-1-methyl-2-phenyl-4H-pyrrolo[1,2-a]benzimidazol-3-yl)- (9CI) (CA INDEX NAME)

PAGE 1-A

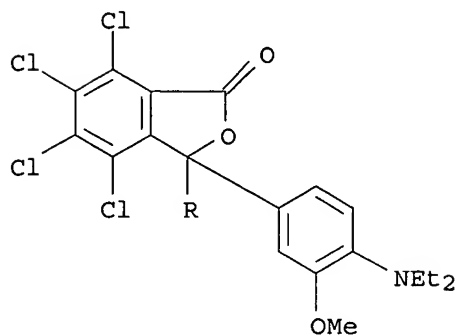
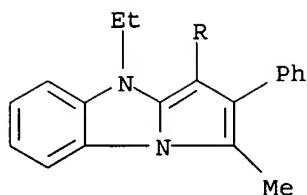


PAGE 2-A



RN 76823-53-5 HCAPLUS

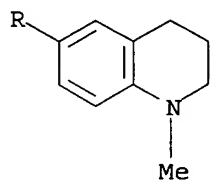
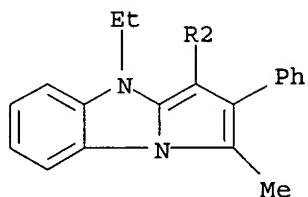
CN 1(3H)-Isobenzofuranone, 4,5,6,7-tetrachloro-3-[4-(diethylamino)-3-methoxyphenyl]-3-(4-ethyl-1-methyl-2-phenyl-4H-pyrrolo[1,2-a]benzimidazol-3-yl)- (9CI) (CA INDEX NAME)



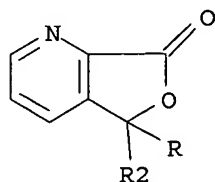
RN 76840-24-9 HCAPLUS

CN Furo[3,4-b]pyridin-7(5H)-one, 5-(4-ethyl-1-methyl-2-phenyl-4H-pyrrolo[1,2-a]benzimidazol-3-yl)-5-(1,2,3,4-tetrahydro-1-methyl-6-quinolinyl)- (9CI)  
(CA INDEX NAME)

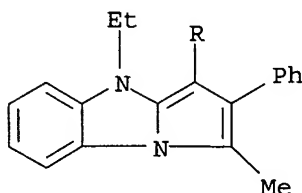
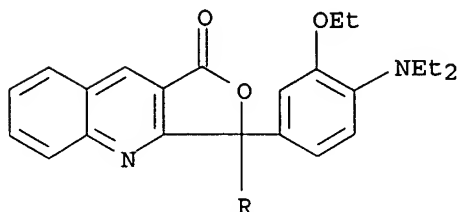
PAGE 1-A



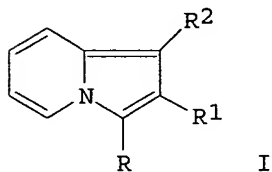
PAGE 2-A



RN 76840-38-5 HCAPLUS  
 CN Furo[3,4-b]quinolin-1(3H)-one, 3-[4-(diethylamino)-3-ethoxyphenyl]-3-(4-ethyl-1-methyl-2-phenyl-4H-pyrrolo[1,2-a]benzimidazol-3-yl)- (9CI) (CA INDEX NAME)



L52 ANSWER 7 OF 7 HCAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 1978:89581 HCAPLUS  
 DOCUMENT NUMBER: 88:89581  
 TITLE: Hetarylation of indolizines  
 AUTHOR(S): Sheinkman, A. K.; Zherebchenko, V. I.; Stupnikova, T. V.; Portsel, E.; Klyuev, N. A.  
 CORPORATE SOURCE: Dnepropetr. Inzh. Stroit. Inst., Dnepropetrovsk, USSR  
 SOURCE: Khimiya Geterotsiklicheskikh Soedinenii (1977), (11), 1510-14  
 CODEN: KGSSAQ; ISSN: 0132-6244  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Russian  
 OTHER SOURCE(S): CASREACT 88:89581  
 GI



AB Hetarylation of 2-methylindolizine I (R = R2 = H, R1 = Me) by quinoline and isoquinoline in the presence of BzCl gave in addition to I R = PhCO, R1 = Me, R2 = H), 60 and 33% I (R = 1-benzoyl-1,2-dihydro-2-quinolyl, 1-benzoyl-1,2-dihydro-2-isoquinolyl). Hetarylations with benzimidazole and imidazole in the presence of Ac2O gave 55% I (R = R2 = 1,3-diacetyl-4-imidazolin-2-yl, R1 = Me) and 93 and 30% I (R = R2 = 1,3-diacetylbenzimidazolin-2-yl, R1 = Me, Ph). Subsequent treatment of the imidazoline and benzimidazoline derivs. gave the corresponding

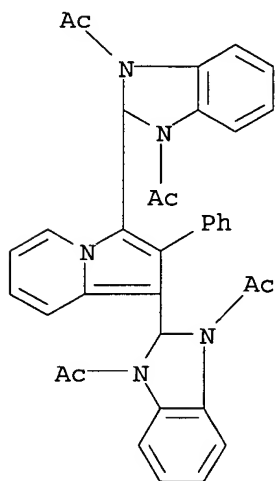
imidazolium and benzimidazolium perchlorates. Similar hetarylations were carried out with benzoxazole and acridine.

IT 65592-74-7P 65592-77-0P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 65592-74-7 HCAPLUS

CN 1H-Benzimidazole, 2,2'-(2-phenyl-1,3-indolizinediyl)bis[1,3-diacetyl-2,3-dihydro- (9CI) (CA INDEX NAME)



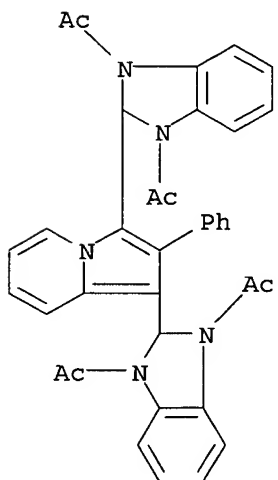
RN 65592-77-0 HCAPLUS

CN 1H-Benzimidazolium, 2,2'-(2-phenyl-1,3-indolizinediyl)bis[1,3-diacetyl-,  
diperchlorate (9CI) (CA INDEX NAME)

CM 1

CRN 65592-76-9

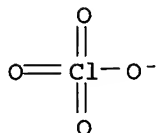
CMF C36 H29 N5 O4



ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

CM 2

CRN 14797-73-0  
CMF C1 O4



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